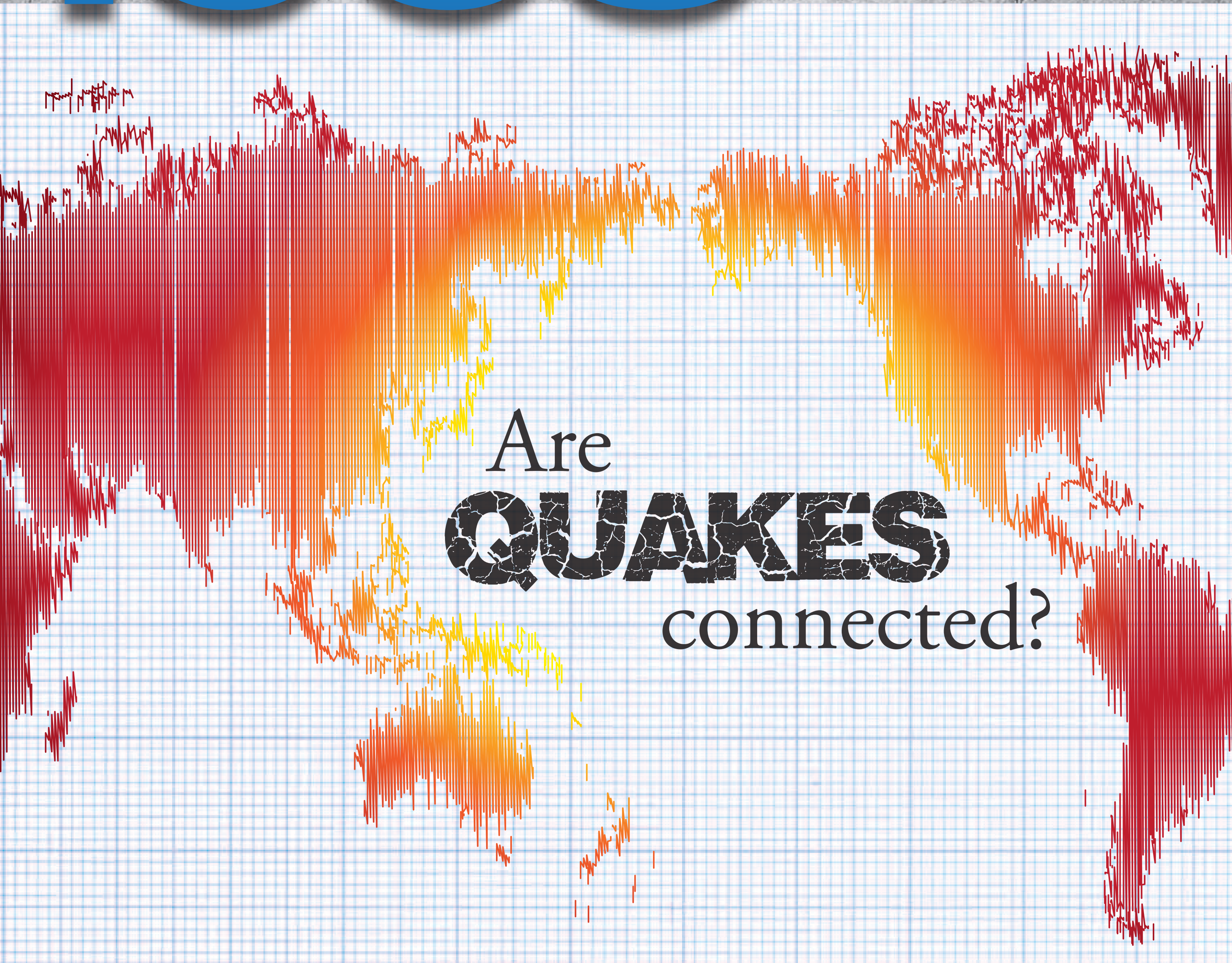
Los Alamos Science and Technology Magazine | April 2014

1663



Are QUAKES connected?

Los Alamos
NATIONAL LABORATORY
EST. 1943

A fancifully false-colored photograph (not a drawing) taken through a scanning electron microscope shows a "forest" of Los Alamos-grown gold nanowires. Both the "trunks" and "leaves" are made of gold. (See "Growing Nanowires" on page 8.)

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1663

LOS ALAMOS SCIENCE AND TECHNOLOGY MAGAZINE

Features

Spotlights

About the Cover:

Predicting earthquakes is a notoriously intractable problem, largely because scientists don't have a firm understanding of the combination of factors that cause them. Recent evidence has shown that quakes tend to cluster in time, over very large distances, implying that large quakes may trigger other large quakes (not just the usual local aftershocks). Now, experiments and simulations at Los Alamos suggest what is going on beneath the surface to cause existing stress points, after being subjected to seismic waves from a prior quake, to fail, thereby producing new earthquakes sooner than they would have occurred otherwise. (See "About to Crack" on page 14.)

About Our Name:

During World War II, all that the outside world knew of Los Alamos and its top-secret laboratory was the mailing address—P. O. Box 1663, Santa Fe, New Mexico. That box number, still part of our address, symbolizes our historic role in the nation's service.

About the LDRD Logo:

Laboratory Directed Research and Development (LDRD) is a competitive, internal program by which Los Alamos National Laboratory is authorized by Congress to invest in research and development that is both highly innovative and vital to our national interests. Whenever *1663* reports on research that received support from LDRD, this logo appears at the end of the article.

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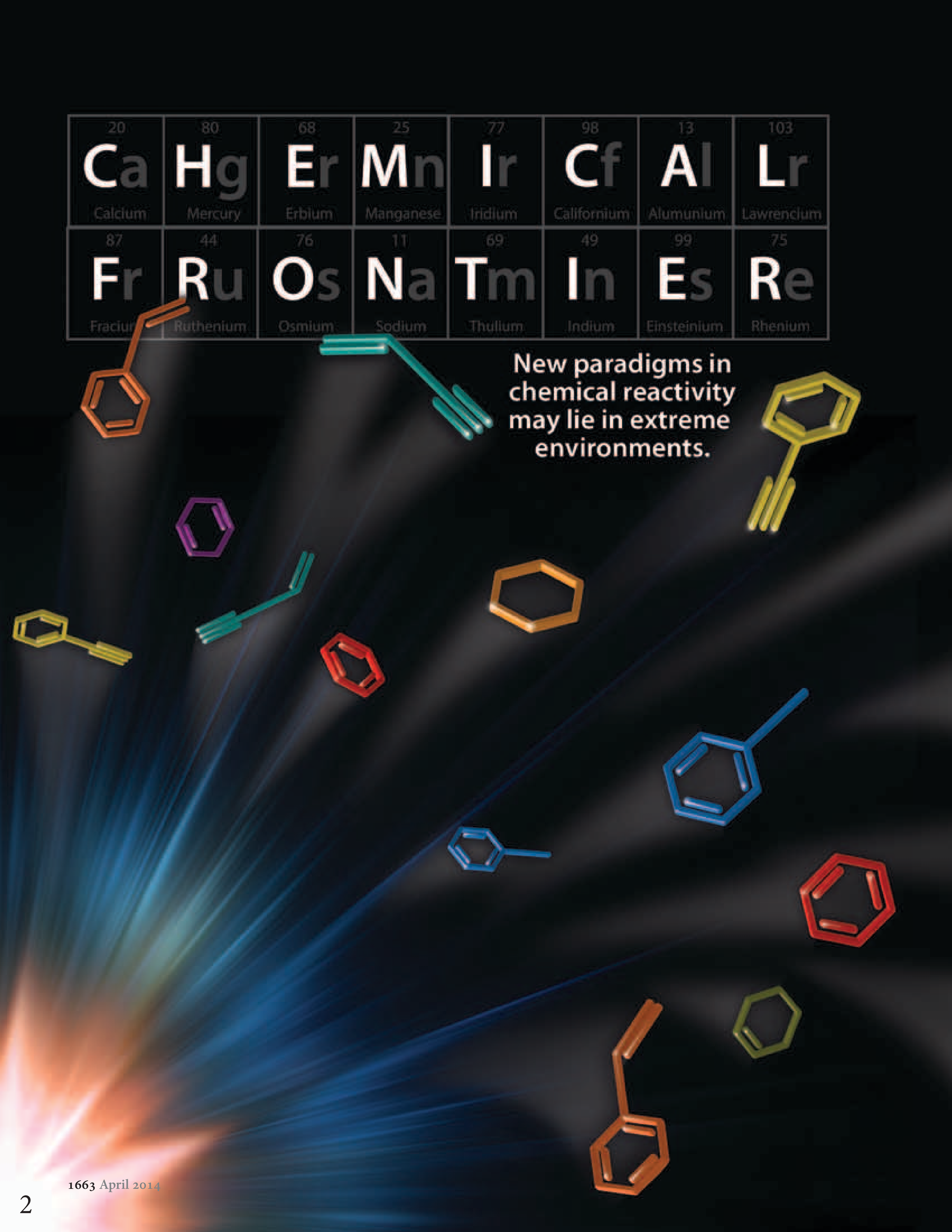

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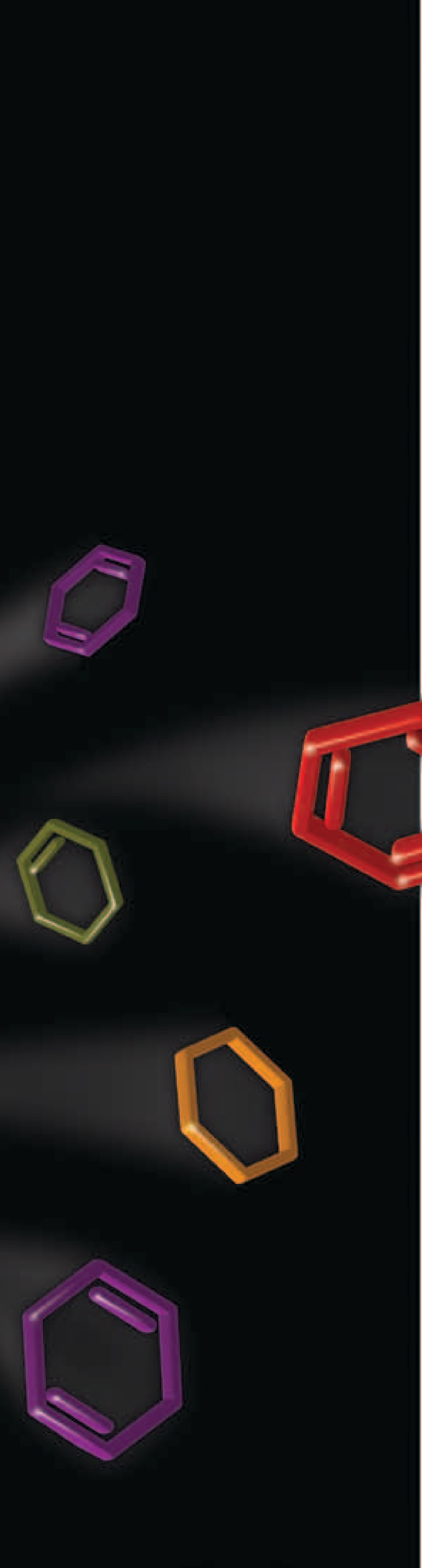
New paradigms in chemical reactivity may lie in extreme environments.



IMAGINE THE PENT-UP FURY OF A POWERFUL EXPLOSIVE the instant before it explodes and how extreme the conditions must be inside to send a blast wave of deafening noise, searing heat, and crushing pressure tearing through the air. In the interior of a high explosive that's reacting, temperatures will soar to thousands of degrees centigrade and pressures will climb upwards toward a million atmospheres. Within this fleeting but hellish internal environment, chemical transformations take place that can't take place anywhere else, involving unique molecular states that scientists are still trying to understand and leading, in some cases, to the creation of novel molecules that should never form according to the guiding principles of general chemistry.

Welcome to the world of shock-induced chemistry. Like the wild American West of days long gone, this world is a wide-open frontier—a chemical frontier of unknowns, governed by its own set of rules. Because of the environmental extremes, molecules on the frontier are slammed together with great energy and squeezed atypically close to one another at very high temperatures, allowing them to undergo reactions that would simply never happen under more benign conditions.

Intrigued by these reactions and their molecular offspring, Los Alamos researcher Dana Dattelbaum and her colleagues have staked a claim on the frontier. Their research has several goals, including gaining a comprehensive understanding of how explosives (or other materials) react when shocked and defining the rules so that new molecules can be designed. Another effort explores how extremely high temperatures and pressures, regardless of how they are generated, can be used to create novel new materials.

Synergystic with the experimental work is the development of computer simulations that shed light on how and why the molecules behave as they do under shock conditions. So far, the programs have been remarkably successful at reproducing the experimental results. Just as important, the simulations are allowing researchers to splice together data taken on vastly different time and distance scales and to construct a consistent picture of how an explosive works. This raises the possibility that someday soon computers will do much of the exploring and will be able to guide the experimentalists down promising research paths.

Getting to know you

Humankind has tinkered with explosive compounds for more than a millennium—references to gunpowder date to 9th century China—yet researchers still don't have a firm understanding of the chemistry that drives the explosion.

What is known is that the explosion is initiated by an impulse, either mechanical or electrical, that sends a shock wave racing through the material at a few thousand meters per second. Ahead of the shock wave lies the undisturbed explosive material at ambient conditions, while behind the shock wave front, or simply the front, is a high pressure, high temperature environment that compresses and instigates the burning of fresh material overrun by the front—the chemical-reaction zone. Through a series of chemical reactions, the high-bond-energy, marginally stable explosive molecules are broken down into stable, lower-bond-energy molecules, such as solid carbon or gaseous carbon monoxide, carbon dioxide, nitrogen, and water vapor. Energy is released in the form of heat and fast-moving reaction products, which increases the pressure and temperature behind the front.

In a non-explosive material, the energy released is either insufficient or released too slowly to sustain the shock, so that the pressure decreases behind the front even as reactions continue. The initial shock wave dies out. But in an explosive material, the

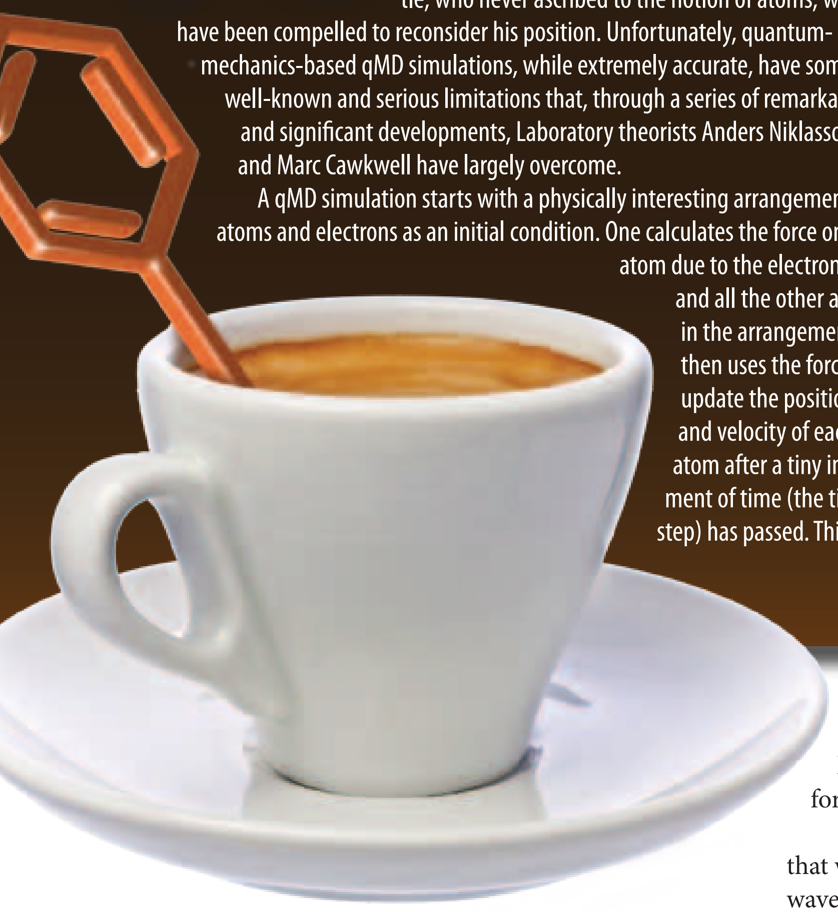
Latte

By simply following the atoms as they move about, a quantum molecular dynamics (qMD) simulation can reproduce and predict the properties of a material so well that even Aristotle, who never ascribed to the notion of atoms, would have been compelled to reconsider his position. Unfortunately, quantum-mechanics-based qMD simulations, while extremely accurate, have some well-known and serious limitations that, through a series of remarkable and significant developments, Laboratory theorists Anders Niklasson and Marc Cawkwell have largely overcome.

A qMD simulation starts with a physically interesting arrangement of atoms and electrons as an initial condition. One calculates the force on each atom due to the electrons and all the other atoms in the arrangement, then uses the force to update the position and velocity of each atom after a tiny increment of time (the time step) has passed. This procedure is repeated over many thousands of time steps until the desired simulation time is reached. Insomuch as the initial arrangement of atoms reflects their configuration in a real material, the collective response of the atoms reveals the material's behavior.

Typically, the number of calculations needed to determine the atomic forces increases precipitously with the number of atoms and electrons in the simulation, and even on the fastest supercomputers a simulation can very quickly become intractable. Research groups often find themselves running qMD simulations with fewer than 100 atoms, severely limiting the types of behaviors that can be studied.

Now the inter-atomic forces are calculated in qMD from the potential energy of the positively-charged atoms and swarming, negatively-charged electrons, with the energy carried by the electromagnetic field generated by those particles. In turn, the potential energy is calculated in a sort-of numerical yin-yang by first making a good guess of the overall electromagnetic field, then figuring out the quantum state of electrons within that field, and finally by checking



liberated energy exceeds what is needed. The initial disturbance becomes a detonation wave, essentially a shock wave that continues to be driven by the chemical reactions occurring behind the front as the front races through new material. The reaction products cause the material to catastrophically blow apart.

This broad-brush description, while interesting, lacks detail. How exactly does the explosive material burn? By which reactions? At what rates? How much energy is released and how quickly? How are non-energetic molecules affected by the shock wave, and what kind of chemistry do they participate in? If the composition of the explosive is modified, how will that affect the sensitivity and the performance of the explosive? Scientists have few answers to these questions.

"We know the starting molecules and have some idea of the final reaction products based on chemical equilibrium," says Dattelbaum. "Other than that, we know very little about the shock-induced chemical reactions behind the front and almost nothing about the details. We don't even know the general principles that are at work. That makes for challenging, incredibly exciting research."

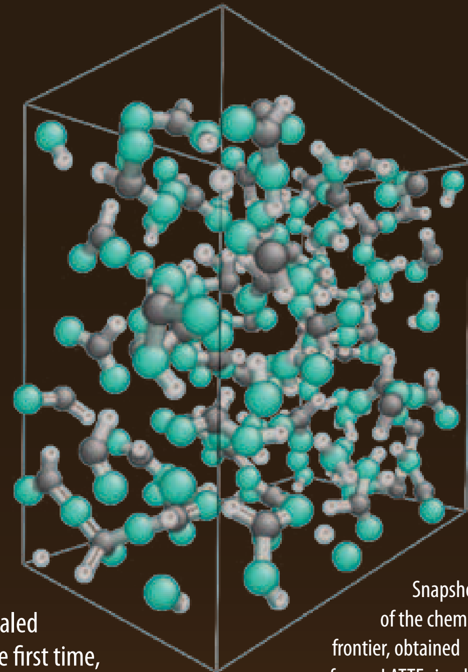
The research is not just exciting; it's necessary. Consider that with a velocity of a few kilometers per second, a shock wave will propagate on the order of several meters in the few milliseconds it takes for the material to explode. Thus, the shock will interact with and affect material structures on every length scale, from the atomic-scale crystal lattice to the micron-scale crystal grains, up to and including bulk-scale cracks, voids, material interfaces, and domains. In particular, it affects and is affected by structures on the sub-millimeter, or mesoscopic, scale—the same structures that affect and control bulk material properties such as strength, the propagation of cracks, alloy properties, etc. Understanding how an explosive works is tied to the much broader picture of what makes materials "work."

Unfortunately, the physics community doesn't have a firm grasp on the physics of the mesoscale and has had only limited success simulating materials on that scale. That may no longer be the case, however. In a significant breakthrough, Los Alamos theorists Marc Cawkwell and Anders Niklasson have been able to vastly increase the size of molecule-based to see that the field produced by this electron state is consistent with the assumed initial field. New guesses are refined over and over until an optimum potential is achieved. The process is known as self-consistent-field (SCF) optimization. It needed to be done for every time step, and it was one of the computational bottlenecks of a qMD simulation.

Niklasson and Cawkwell recognized that by introducing an auxiliary electron population to the calculations along with a slightly modified formulation of the inter-atomic forces, the SCF optimization and its gluttonous eating of computer cycles could be eliminated entirely from the computer code. Furthermore, the new formulation was amenable to "fast solver" techniques that slashed the number of numerical operations needed to solve the force equations.

When all the i's were dotted and the t's crossed, the two theorists had demonstrated a turbocharged simulation method that was just as accurate as an "exact" qMD formulism. Most significantly, they proved that it was possible to run a qMD simulation with millions of atoms on large parallel supercomputers with no loss of accuracy. Their work was selected as an Editor's choice of the prestigious *Journal of Chemical Physics* for 2012.

Niklasson and Cawkwell have developed a new quantum molecular-dynamics code, LATTE (Los Alamos Transferable Tight-binding for Energetics), which has already been used to predict the chemical reactivity and spectral features of organic materials under shock conditions. They were able to build their material with an unprecedented number of atoms and so run qMD simulations that revealed large-scale material behaviors. For the first time, reserchers were able to verify and correlate experimental results obtained under vastly different conditions. Not only is this leading to a unified picture of how an explosive works, but in a more general context, to a greater understanding of materials that even Aristotle would have relished.



Snapshot of the chemical frontier, obtained from a LATTE simulation of shock-induced chemical reactions in liquid formic acid.

simulations of materials without breaking the computational bank, setting the stage for a quantum-based molecular dynamics simulation of mesoscale physics. (Read about their work in "Latte" above.)

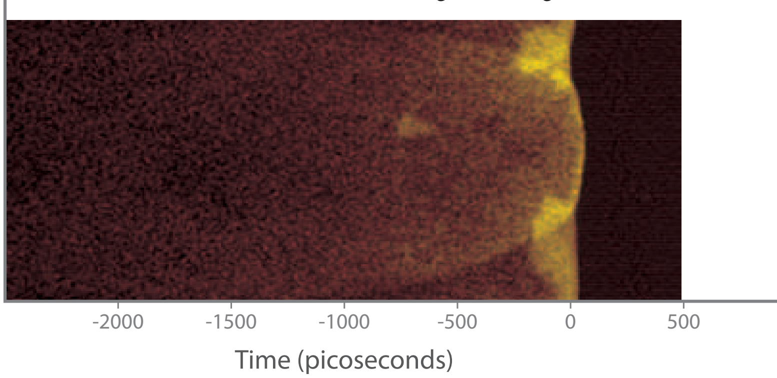
Explosive program

Dattelbaum's team is trying to fill in many of the gaps in our understanding of complex materials by studying simple molecules, both energetic and inert, and removing microstructure from the equation. The team uses two methods to launch well-defined shock waves into the materials—a unique, large-bore, two-stage gas gun and high repetition-rate, pulsed lasers. They then use a variety of diagnostics to quantify the chemistry that occurs following shock compression.

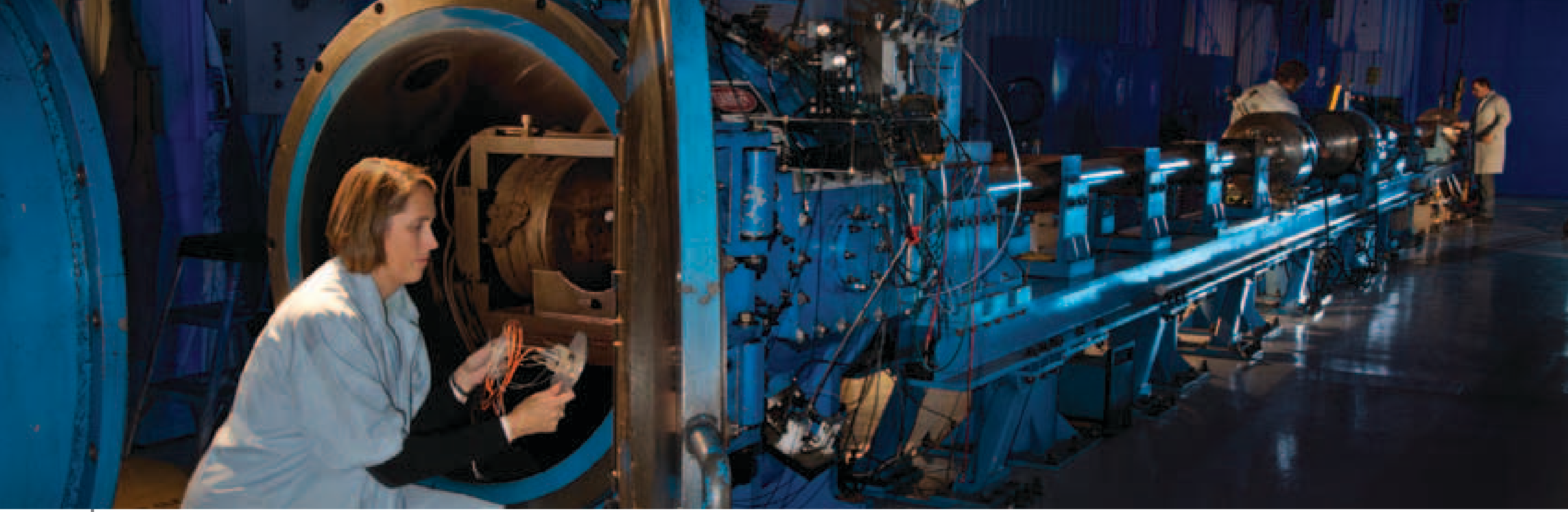
In the first method, a large gas-driven gun fires a projectile into a plate covering the material of interest, which gets shocked by the collision. Something on the order of 100,000–1,000,000 atmospheres of pressure (roughly between 7 and 70 percent of the pressure at the center of the earth) can be achieved, with the pressure remaining at some high level for several millionths of a second.

In the second experimental method, the team focuses a high-power laser on a metal plate that is bonded to the material. The plate gets very hot very quickly and rapidly expands, sending a shock wave into the material. The maximum pressure achieved is tied to the laser power and overlaps what can be achieved with the gas gun. In contrast to the gas gun experiments, the pressure behind this front reaches its maximum in just a few picoseconds (10^{-12} seconds), then fades relatively quickly. Using both methods, the group is able to obtain information about both the short- and long-time evolution of the shock-induced chemistry.

By using embedded electromagnetic gauges, the team is able to study reactions occurring behind the front on timescales ranging from tens of nanoseconds to several microseconds. First used by Russian scientists in the 1960s, the tiny, foil-like metal sensors are inserted directly into the explosive. A magnetic field is generated around the sample by an electromagnet, so when the shock wave compresses the material, the metal sensors move through the magnetic field,



A density plot of a shock front, similar to what one might see using proton radiography, from a large simulation using several million molecules. Unreacted material is dark brown (positive times). The yellow regions are the high density detonation shock front, followed by regions of darkening brown as the reaction completes and the product gases expand.

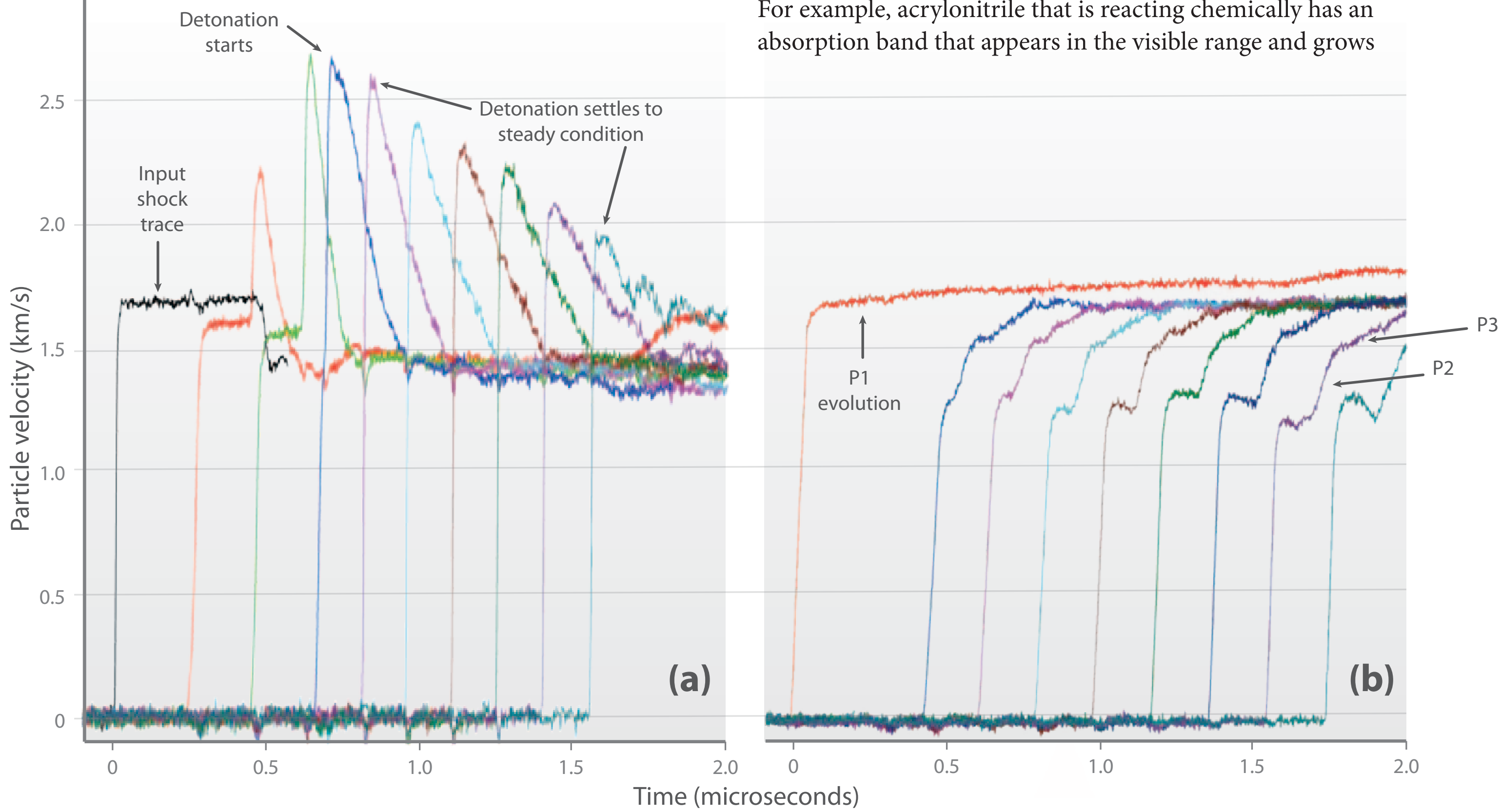


Los Alamos scientist Dana Dattelbaum, seen here at the end of a large gas gun (which extends backwards all the way to the rightmost researcher). The gas gun is one of several pieces of equipment used by Dattelbaum and co-workers Steve Sheffield, Shawn McGrane, Nhan Dang, and Josh Coe in the study of shock phenomena.

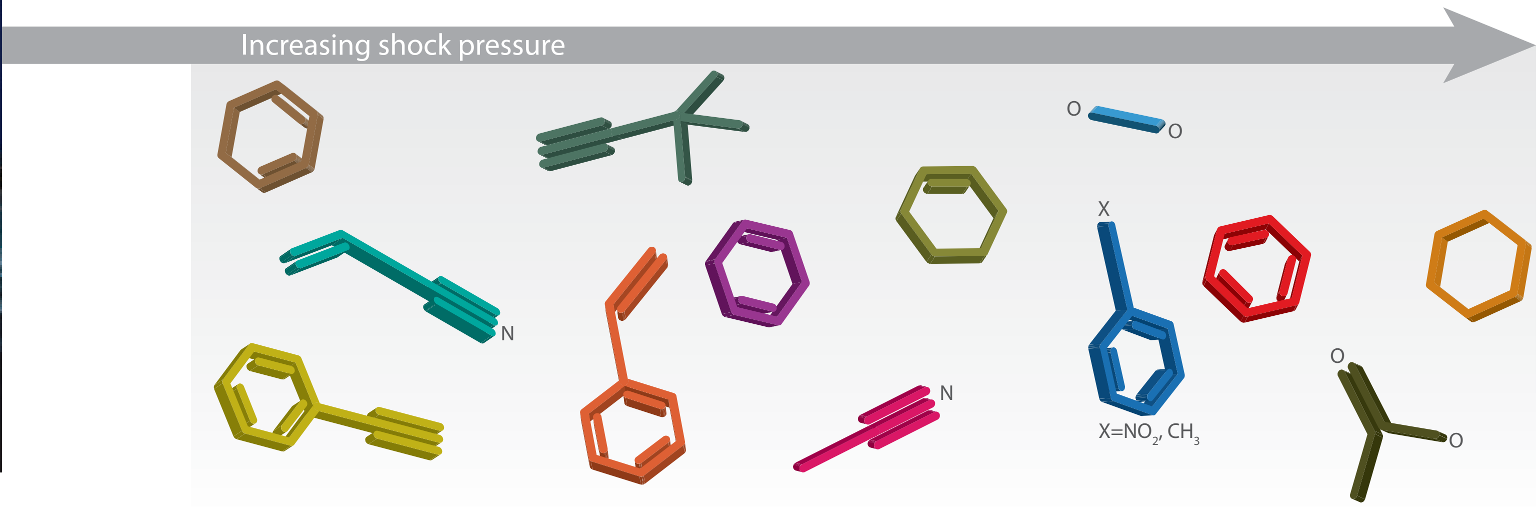
generating a voltage that is proportional to the material's mass or particle velocity. The technology was perfected at Los Alamos, which is currently the only place in the United States where it's used. When combined with other diagnostics, such as optical velocimetry, the team is able to measure the wave dynamics associated with reaction chemistry, including the buildup to detonation, and to probe the reaction zone behind the detonation front during a brief time window.

Of note is that different materials react in different ways under shock loading. In contrast to explosives, many materials, such as the prototypical organic molecule benzene, and many of the polymers used in defense and weapons applications do not release enough energy to drive the shock front when they react. Furthermore, the reactions result in products that are denser than the starting material.

Studying the various reactions often requires a diagnostic that can probe the system on trillionth-of-a-second timescales. Absorption and vibrational spectroscopy fit the bill. For example, acrylonitrile that is reacting chemically has an absorption band that appears in the visible range and grows



(a) The graph shows data from a series of gauges inserted at specific points within nitromethane, a water-like, yet flammable, liquid. As the shock wave moves through the series, each gauge produces a trace of particle velocity, which is proportional to the pressure. The pressure behind the front is seen to build above that of the initial shock (black trace) until, at detonation, the burning of fresh material becomes the driver of shock propagation. (b) Dattelbaum and her team have discovered evidence for intermediate products, such as polymers, forming behind the shock front from simple molecules. Phenylacetelyne, shown here, is seen to produce a pronounced three-wave structure, indicating an intermediate is formed on the way to the final products.



Dattelbaum's group has established an order of shock reactivity for simple chemicals, which they include in what they call their "shock chemistry handbook." As the pressure from a shock wave increases (arrow), the energy available for bond-breaking increases and different kinds of molecules become reactive. The general sequence of bond-breaking begins with carbon-carbon triple bonds (at roughly 5 gigapascals of pressure), and progresses through, for example, carbon-carbon double, carbon-nitrogen triple, oxygen-oxygen single, and carbon-carbon single bonds (at greater than 20 gigapascals).

as a function of time as the chemical conversion proceeds. By combining ultrafast absorption spectroscopy with shock compression techniques, the team has been able to directly measure changes in absorption properties of the chemical intermediates.

Exciting research

Thanks to the healthy experimental program, Dattelbaum and colleagues are slowly writing the book on the chemistry behind the front: what it takes to initiate chemical reactions, how the reactions proceed, the stability of the reaction products, etc. Then in conjunction with state-of-the-art with computer simulations, more complicated reactions can be analyzed in terms of the guiding principles established for the basic reactions.

"If the principles of shock-driven reactivity were better understood, including how they translate to explosive crystals, they may be applied to the design of insensitive explosives," says Dattelbaum, referring to materials that detonate and explode normally, but which are difficult to initiate. At the national laboratories, a goal is to create a new type of insensitive explosive that is nearly impossible to initiate except under very specific and controllable circumstances. "That's the holy grail, because such a material would greatly enhance the safety margin for all applications of chemical explosives, from ammunition to demolition, mining, and even nuclear weapons."

One could envision creating this new insensitive explosive by designing the first bond-breaking step to have a high-activation barrier, or by incorporating functional groups into the explosive molecule that will hold the molecule together, allowing it to break only under higher pressure and temperature conditions. The molecule overall would still decompose energetically to detonation products once initiated.

At present, there isn't a research group in the world that can accurately predict the sensitivity of an explosive formulation *a priori*. But the team is closer than ever in being able to predict thresholds for shock-driven reactions, including the shock sensitivities of explosive molecules, and is quantifying reaction rates as a function of shock pressure and temperature. Dattelbaum is confident that they will soon be able to recognize promising candidates for an insensitive explosive.

Lastly, Dattelbaum would like to see a robust program of novel-material research and development. Novel polymers are already being considered for body armor, and shock-wave dissipating foams have been developed that absorb the shock of a nearby explosion and so protect structures from a terrorist threat. Those novel materials were not created in the throes of an explosion, but extreme conditions can be used to create new states of matter and new molecules that are semi-stable under normal conditions. Could shock-induced chemistry or other extreme techniques become a means to produce the novel materials of the future?

We'll have to wait to see. Still, these explorations of the chemical frontier could not be more timely or appropriate. New techniques that enable pioneering scientists to probe reactions at shorter length and time scales and in harsh conditions are being combined with molecular dynamics simulations that can predict the chemistry and elucidate experimental results. The prospects for interesting science are almost as great as the desires of the scientific frontiersmen to bring the chemistry from behind the front to the fore. LDRD

—Jay Schecker

GROWING NANOWIRES

Tiny semiconducting strings for virtually every purpose

"THERE IS THIS REMARKABLE HISTORY in which the semiconductor components of computer chips have gotten smaller each year, with performance improving along with the miniaturization," says Jennifer Hollingsworth, a Los Alamos materials chemist specializing in nanotechnology. Hollingsworth constructs quantum dots and nanowires, the ultimate in miniature semiconductors, with potential uses that reach far beyond computer chips. "But we're going about it from the opposite direction: building tiny semiconducting structures from the bottom up."

Hollingsworth is the co-science leader of the nanowire integration focus area within the Center for Integrated Nanotechnologies (CINT), a joint enterprise between Los Alamos and Sandia national laboratories in New Mexico. Like four other Nanoscale Science Research Centers, CINT is a premier Department of Energy (DOE) user facility for interdisciplinary research that serves as the basis for a national nanoscience initiative, encompassing new science, new tools, and new computing capabilities.

That's where Hollingsworth and her nanoscale semiconductors fit in. Renowned for finding a solution to a long-standing "blinking" problem with quantum dots (switching off and on), she has recently turned her attention to novel semiconductor nanowires and new methods for growing them. She invented a method that would enable unprecedented control over nanowire fabrication in solution, promising lower cost and lower-temperature growth and processing. At the same time, the wires would be of high quality with structures designed to suit particular applications—important attributes for making commercially viable nanowire components.

"At that point," Hollingsworth says, "a lot of technological progress will follow." Indeed, semiconductor nanowires are expected to bring about transformative improvements to solar cells, rechargeable batteries, thermoelectric energy converters, biomedical devices, computers, sensors, and a host of other electronics.

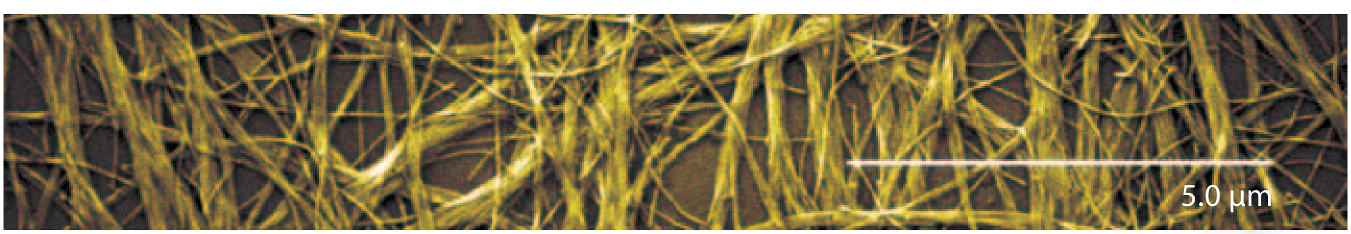
What's in a wire?

Quantum dots and nanowires owe their special properties partly to the semiconductor materials they are made from and partly to their miniscule size. The properties of semiconductors—whether in bulk, miniaturized, or nanoscale—are derived from their internal energy structure: Most of their electrons possess energies within a particular range known as the valence band, while a few are in a higher-energy range known as the conduction band, with an unoccupied energy gap in between. In general, the greater the number of valence-band electrons that can be manipulated into jumping the energy gap to the conduction band, the more electrical current the material will support.

In one of a computer chip's many transistors, for example, a voltage can be temporarily applied to supply the energy needed to populate a semiconductor's conduction band in such a way as to create a new conducting path. This essentially has the effect of flipping a switch, but with no moving parts, so it allows the computer to rearrange its own circuitry to perform different calculations and execute a variety of programs. Outside of computing, semiconductivity is also the basis of many other important technologies, including LED-based lights and lasers, solar cells, and a number of ubiquitous circuit components.

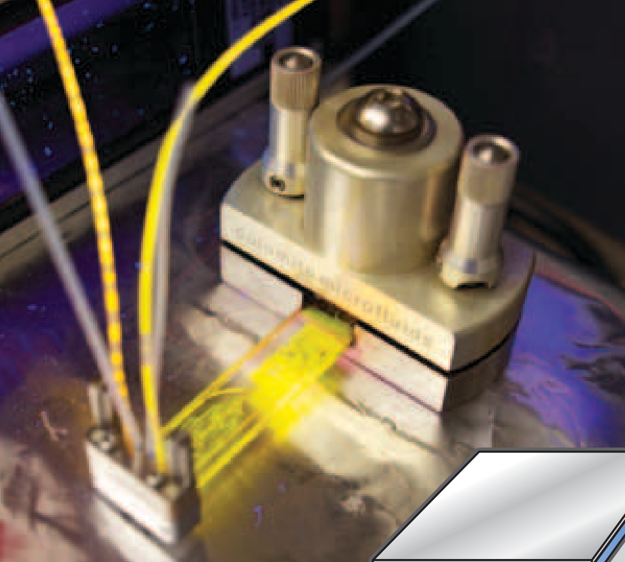
In terms of size, nanoparticles (dots or wires) are often just nanometers (10^{-9} meter) in diameter, less than one-ten-thousandth the diameter of a human hair. At that small size, electrons experience something called quantum confinement, in which the physics that governs their behavior is altered because they are "squeezed" by their confined space. The effect adjusts the structure of the semiconductor's energy bands and the gap between: the smaller the nanoparticle, the greater the energy gap. Therefore a desired energy gap can be obtained simply by constructing a nanoparticle of the correct size. Furthermore, because a larger-than-usual fraction of the atoms or molecules in a nanoparticle reside on its exterior surface, their quantum "surface physics" comes into play much more than it would in a larger object. Among other things, this makes quantum dots and nanowires extremely sensitive to the presence of small entities nearby, making them useful for detecting particular molecules in chemical and biological applications.

Taken together, semiconductivity and quantum confinement allow scientists and engineers to meet an incredible variety of technological challenges. Want a faster microprocessor? Cram an enormous number of tiny nanowire-based transistors onto your chip. Want a solar cell that draws more energy from sunlight? Arrange your nanowires to maximize



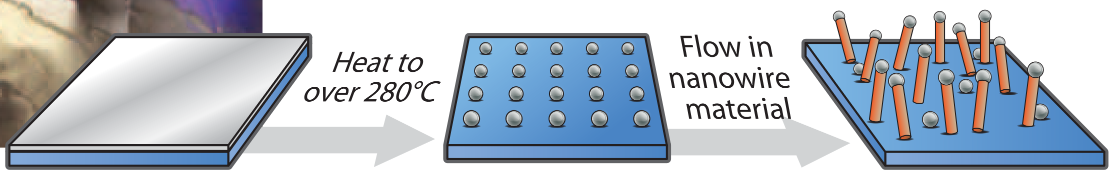
Electron micrograph images of nanowires in the "spaghetti" and "forest" configurations. (Above) These cadmium selenide nanowire strands and "ropes" were grown in the solution phase and deposited on a solid substrate, or surface. (Opposite page) This false-color electron micrograph shows gallium nitride nanowires on a silicon substrate, designed to emit visible and ultraviolet light for laser applications and other uses.

CREDIT: (above) Jennifer Hollingsworth's lab/LANL; (opposite) Lorelle Mansfield/NIST



(Left) The flow-SLS device (yellow), with fluid inlet and outlet tubes (also yellow), is set inside a stainless-steel mounting (center) that preheats incoming fluid and maintains a constant temperature throughout the growth region inside. (Below) The Los Alamos microfluidic flow-SLS nanowire growth method, like the more common vapor-phase method, starts with a substrate in a reaction chamber. The substrate (blue) is coated with a thin bismuth film (white); upon heating, the film breaks into small droplets which will catalyze the nanowire growth. When the nanowire material is flowed into the reactor via a carrier solvent (along with some necessary additives), it enters the catalyst droplets and subsequently crystallizes onto the interface between the droplets and the substrate below, thereby growing the nanowires from the bottom up.

CREDIT: Jennifer Hollingsworth/LANL



light absorption and minimize reflection. Want to detect an individual protein molecule associated with cancer? Design the energy levels of a nanowire device to populate its conduction band in response to electrical charges on the protein's binding surface. The possibilities truly abound—if controlled nanoparticle synthesis can be made cost effective at the industrial scale.

Tale of two syntheses

Semiconductor nanowires may prove more versatile than quantum dots for some applications. Whereas quantum dots are nano-sized in all three dimensions, nanowires are nano-sized in only two. They have one long dimension, typically 20 to 1000 times longer than the wire's diameter. And because of their long dimension, they can be manipulated, anchored on the ends, and arranged in different configurations to suit the needs of different applications. When used in solar cells, for instance, nanowires offer a significant advantage over quantum dots. The wire shape is better for conveying photoelectrons (individual units of solar electricity) into whatever external circuit the solar cell is connected to before they disappear by ineffectually recombining with the electrical charge "holes" left behind during their production.

There are two primary methods for making nanowires, each with its pros and cons. Unlike most other nanotech facilities, Hollingsworth points out, CINT does both.

One method, called vapor-liquid-solid synthesis, or vapor-phase synthesis, starts with tiny nanocluster droplets of a liquid metal catalyst, such as liquid gold, arranged on a substrate (surface). A semiconducting material such as silicon, from which the nanowire will be made, is then injected in vapor form into the chamber housing the substrate. The vapor diffuses into the liquid metal droplets until it supersaturates, at which point it crystallizes onto the substrate at the base of the droplet. As the process continues, each newly deposited bit of crystal builds upon the last, causing a nanowire to grow vertically, elevating the catalyst droplet as it grows. When a "forest" of nanowires (so named because they stand parallel to one another like trees) grows to the desired nanowire height, the vapor inflow is shut off.

Jinkyoung Yoo is a colleague of Hollingsworth's at CINT who specializes in growing nanowires by vapor-phase synthesis. This method allows him to produce extremely high-quality nanowires—pure of composition and defect-free—in the forest arrangement that's favored for use in solar collectors and electronic devices. The vapor-phase method also permits him to make the wires "heterostructured"—alternating between two opposing types of semiconducting materials—by flowing the vapors of each material into the chamber in an alternating sequence. This, too, is important for electronics applications, which require joining the two types of semiconductors, *p*-type and *n*-type, to make what's called a *p-n* junction. (The letters indicate positive and negative, referring to their tendency to either accept or donate electrons. At a *p-n* junction, the *n*-type semiconductor donates electrons to the *p*-type semiconductor.)

"With vapor-phase growth, you can make *p-n* junctions in individual heterostructured nanowires," says Yoo, "and you can make more complex logical elements like transistors by crossing those wires." Indeed, vapor-phase is the method of choice for anyone wanting enough control over the growth process to produce forest-style, heterostructured nanowires for electronic devices. But the process is slow, and it's expensive due to the high-purity semiconductor starting materials needed. Those starting materials are both toxic and flammable, adding to the expense with the required safety precautions. For these reasons, although vapor-phase has already proven its value at the laboratory scale and in industry R&D—permitting fine-tuning of composition, conductivity, energy band spacing, and so on—it may prove impractical at the production scale, when expense becomes the driving factor.

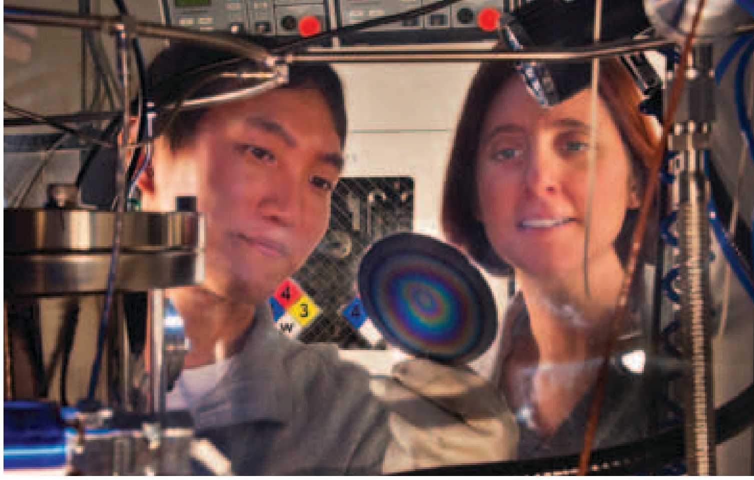
The other common method, called solution-liquid-solid synthesis, is a type of solution-based synthesis that's less expensive and scales up easily. The nanowires can be grown in large batches in solution. Like vapor-liquid-solid growth, molten metal nanocrystals are used as a growth catalyst. Here, however, they are immersed in a solvent, so that when semiconductor precursor chemicals are released into the solution, they become incorporated into the liquid metal particles until the semiconductor nucleates and grows into a nanowire structure. The solution-based growth process is about a thousand times faster than vapor-phase synthesis, taking as little as seconds or minutes to complete. Once finished, the nanowires have the additional benefit that, because they're soluble, they can be sprayed, dip-coated, or painted onto a surface. For certain applications, this flexibility, in addition to the potentially large batch sizes, equates to low cost.

But of course there's a catch. With the speed and relative ease of growth in solution comes a loss in quality and control. Solution-based synthesis takes place at a lower temperature than vapor-phase synthesis, and that lower temperature can lead to structural defects. Also, instead of slow, consistent growth with a measured and controlled rate of precursor incorporation and removal of byproducts, the concentration of reactants varies throughout the process, with no removal of byproducts. Finally, because the solution method is essentially an all-at-once process, it's impractical to make heterostructured nanowires. So solution-based synthesis scales up to industrial use well, but lacks the precision of the vapor-phase method to create the high-quality, forest-style, heterostructured nanowires required for many applications.

If only there were a way to combine the two.

Best of both worlds

"We needed a way to achieve the controllability of the vapor-flow method while maintaining some of the practical, ease-of-use benefits and lower cost of solution chemistry," Hollingsworth explains. "In other words, we needed



Jinkyoung Yoo and Jennifer Hollingsworth of Los Alamos examine nanowires grown by vapor-phase synthesis in the metal reaction chamber at left.

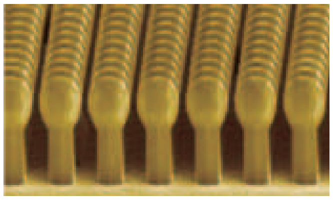
a flow-based solution process that's slow and steady enough to adjust and optimize, with the potential to scale up." The resulting innovation? Flow-based solution-liquid-solid synthesis, or flow-SLS for short.

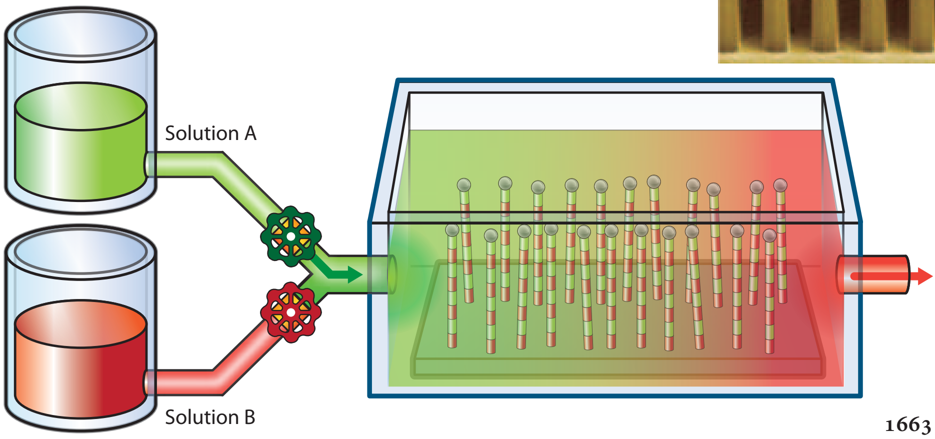
To obtain the necessary level of control, Hollingsworth decided on a microfluidic reactor platform, which recently came to fruition thanks to several postdoctoral researchers. Nick Smith (who has been promoted to Los Alamos research staff) started the effort, which was then perfected by postdoctoral fellow Rawiwan Laocharoensuk, with help from Kumar Palaniappan.

Microfluidics generally refers to the manipulation of fluids flowing in small-volume channels, typically less than a millimeter wide, as in ink-jet printing. In the case of the flow-SLS microfluidic reactor, a thin tube carries the semiconductor reactants (and some coordinating molecules called ligands) in a solvent into a resealable, computer chip-sized chamber. There, the solution flows over a substrate littered with liquid-metal catalyst droplets. The semiconducting material supersaturates the droplets and grows nanowires from the solid surface below them, just like vapor-phase synthesis, and the byproduct-containing solution flows out of the chamber.

Nanowire growth with flow-SLS isn't as rapid as in standard solution-based synthesis, but it provides for a number of reaction parameters that can be carefully dialed up or down

Heterostructured nanowires, in which wire segments made from different semiconducting materials are joined together, can be used in electronic components for a wide range of applications. (Below) In Hollingsworth's solution-based flow-SLS production method, axially heterostructured nanowires—with different semiconducting materials along the length of the wire—are made by alternating the solutions flowing into the reactor. (Right) Again using alternating reactants, but in the vapor phase, Yoo was also able to make radially heterostructured nanowires, in which the differing semiconductors are arranged concentrically like tree rings. Shown here are heterostructured silicon *p-n* junction nanowires (see main article) for use in solar cells.



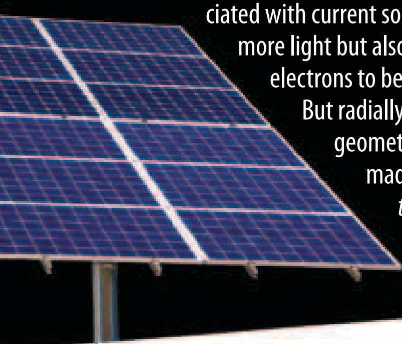


BIG ENERGY
from the littlest wires

Solar Cells

Silicon nanowire solar cells have the potential to achieve better light collection and lower production cost compared to existing silicon solar cells. Bulk, planar silicon cells reflect—and therefore waste—a substantial amount of the incident sunlight, but nanowire forests have been constructed in a way that scatters light from wire to wire, trapping it until it can be absorbed. And because of the gaps between the wires, nanowire solar cells can be produced with much less bulk, and even on less expensive substrates, than existing solar cells.

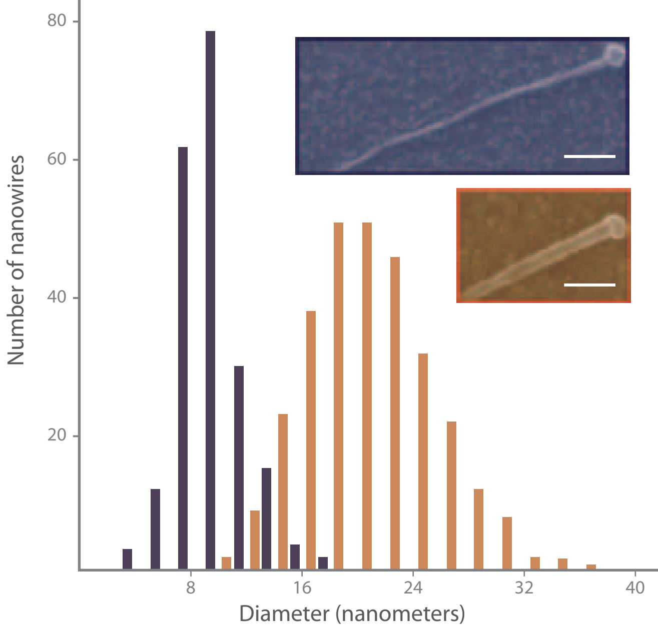
Los Alamos's Jennifer Hollingsworth and Jinkyoung Yoo both contribute to nanowire solar power research. Hollingsworth is working from solution-cast nanowires and relying on their ability to "sensitize" other semiconductors to solar energy. Yoo is constructing radially heterostructured nanowires (see main article) to help resolve a major trade-off associated with current solar cells: Thicker silicon layers absorb more light but also allow more time for solar-produced electrons to be lost in a process called recombination. But radially heterostructured nanowires have a geometric advantage because they can be made *longer* to absorb more sunlight, but *thinner* to reduce the time available for recombination.



Rechargeable batteries

Lithium-ion batteries are already used in phones, computers, electric cars, and just about everything else. Their storage capacity is limited by the amount of lithium that can be held in their anodes, which are currently made from carbon graphite. They could store 10 times more electrical charge (and last 10 times longer) if their anodes were made from silicon instead, but bulk silicon's advantage is also its undoing. Because it draws in so much lithium, its volume swells and contracts during charging and discharging, causing it to fracture. Over several charging cycles, damage accumulates and the storage capacity declines. However, the thin, extruded shape of silicon nanowires can accommodate the volume change without damage, allowing vastly greater storage capacity over many more charging cycles than existing lithium-ion batteries. Former Los Alamos researchers Tom Picraux and Jeong-Hyun Cho achieved several hundred charging cycles of reliable battery performance with many times the energy storage capacity of existing batteries just by optimizing the structural quality of bulk silicon. Yoo is working to raise their success to the next level with nanowire silicon.

With their flow-SLS protocol, Hollingsworth and her team were able to adjust the diameter of the nanowires they produced by varying the thickness of the bismuth film that breaks into catalyst droplets and the rate at which they flow reactants into the microfluidic reactor. Thinner nanowires resulted from thinner catalyst films and faster reactant flow rates. The histogram shows the range of nanowire thicknesses resulting from a relatively thin, 5-nanometer-thick bismuth film. Blue indicates nanowires obtained with a flow rate 10 times faster than that for orange. White lines in the inset micrographs are 100 nanometers long.

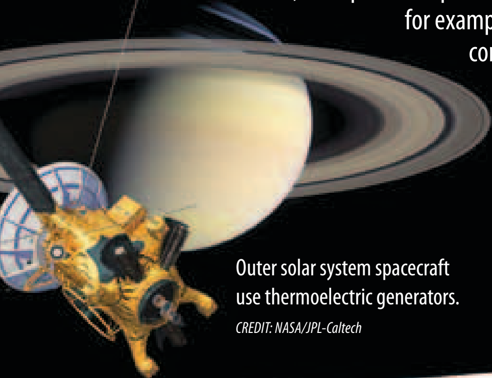


to improve the output. For example, by decreasing the size of the catalyst droplets, adjusting the reaction temperature, and increasing the flow rate, Hollingsworth's team was able to build single-crystal wires 5–8 nm in diameter—well within the useful quantum confinement regime for controlling the semiconductor energy gap. And by injecting an alternating sequence of two different semiconducting materials, they were able to make heterostructured nanowires, as needed for semiconductor electronics and other applications.

Once the flow-SLS process has completed, the wires can be harvested from the substrate and arranged as needed for whatever application is at hand. And because of their solubility, they can be delivered in industrially convenient ways, such as spray-on inks and dip-coatings. So far, solution-liquid-solid growth has produced nanowires more like spaghetti than a forest—but Hollingsworth says that with flow-SLS, a

Thermoelectric devices

When a circuit made from certain materials spans a temperature difference (one end of the circuit is hotter than the other), the thermoelectric effect causes an electrical current to flow. This effect is often exploited in temperature sensors and can be used for very specialized power production applications, such as generating electricity from the heat-producing plutonium cells that power long-range spacecraft. However, existing thermoelectric devices have very low efficiencies and therefore are only useful in a handful of specialty applications. If their efficiencies could be increased, thermoelectrics could generate electricity from waste heat, to improve the performance of a solar panel or a car engine, for example. Nanowires can deliver electrical conductivity without much thermal conductivity, helping to maintain the temperature difference. But very little temperature difference can exist across the tiny length of a nanowire, so Hollingsworth is researching different web-like networks of nanowires to increase the temperature difference they can sustain.



Outer solar system spacecraft use thermoelectric generators.

CREDIT: NASA/JPL-Caltech

Lighting and lasers

Light-emitting diodes, or LEDs, produce light at a much lower energy cost than incandescent and fluorescent sources, but they are expensive to manufacture and have limited emission colors. Here, Hollingsworth focuses on specialized nanocrystal quantum dots that she and her team developed with unique properties that make them particularly useful for light emission. They can serve as the active component in an LED (electrically stimulated to emit light) or perform color conversions from blue light to green, yellow, or red, much like rare-earth compounds do in fluorescent lights and white-emitting LEDs today.

"Unlike solar and battery applications, which are very cost-sensitive, LEDs and other high-efficiency lighting are already expensive anyway," Yoo says. "So even a somewhat costly nanoparticle LED has a good chance of succeeding in industry, as long as it's efficient and delivers the right kind of light."

forest is achievable, too; it's just a matter of properly matching the semiconductor nanowire with its substrate.

In essence, she and her team achieved creative control over the nanowire production process in a relatively inexpensive, versatile, solution-based alternative to vapor-phase synthesis. Their innovation may help usher in an era of bona fide nanowire commercialization. Yoo agrees that flow-SLS is a "really smart way" to make nanowires for various future applications, even though the vapor-phase approach he works on has a substantial head start in R&D.

Nanowired world

Just what kinds of technological breakthroughs would a production-scale nanowire industry bring about? Most people in the nanotech field would jump to computing, noting the potential quantum leap in transistor miniaturization that crossed heterostructured nanowires represent. Others would point to biomedical applications inspired by the availability of tiny sensors. But not surprisingly, at CINT, and within the DOE more broadly, the focus is largely on energy. And the nanowire-energy revolution is just getting started.

Nanowires are almost certainly capable of significantly boosting solar power efficiency and rechargeable battery life. They are also likely to enable much lower-cost lighting than is currently available. (That benefit alone would be worth the effort; lighting amounted to 12 percent of all U.S. electricity consumption in 2011, according to the Energy Information Administration.) Nanowires may even revolutionize thermoelectric devices, which could then be used to harvest electrical energy from any source of waste heat—and virtually all energy production processes, and many other industrial processes, produce wasted heat. Together, these energy-related nanowire applications could drastically reduce the economic and environmental costs of human energy use. (See "Big Energy from the Littlest Wires" above.) Such is the potential for energy advances that persistently entices Hollingsworth, Yoo, and perhaps everyone else in the nano-energy innovation business. It consumes their every thought—almost.

In her small, packed office at CINT, Hollingsworth changes gears. Instead of continuing to describe her flow-SLS research and its potential for solar or thermal energy harvesting, or her quantum dot lighting research, or any of the semiconductor and chemical-synthesis fundamentals that underlie it all—instead of that, she mentions something new. It's another nanoparticle application that she's pursuing: a new nanoparticle to someday simultaneously image and treat cancer by selectively generating both light and heat—to expose and then attack a tumor inside the body—for a controlled kill.

"You know," she says impassively, "instead of chemo."

LDRD

—Craig Tyler

About to Crack

***Los Alamos scientists** are figuring out how to do*

THE DATE WAS FEBRUARY 4th, 1975, and the setting was the city of Haicheng in northern China. On that day, the earthquake science community had a major breakthrough—for the first time ever, an earthquake of catastrophic proportions had been successfully predicted. Roughly a million people were evacuated beforehand and an untold number of lives were saved. There was just one problem: it was a fluke.

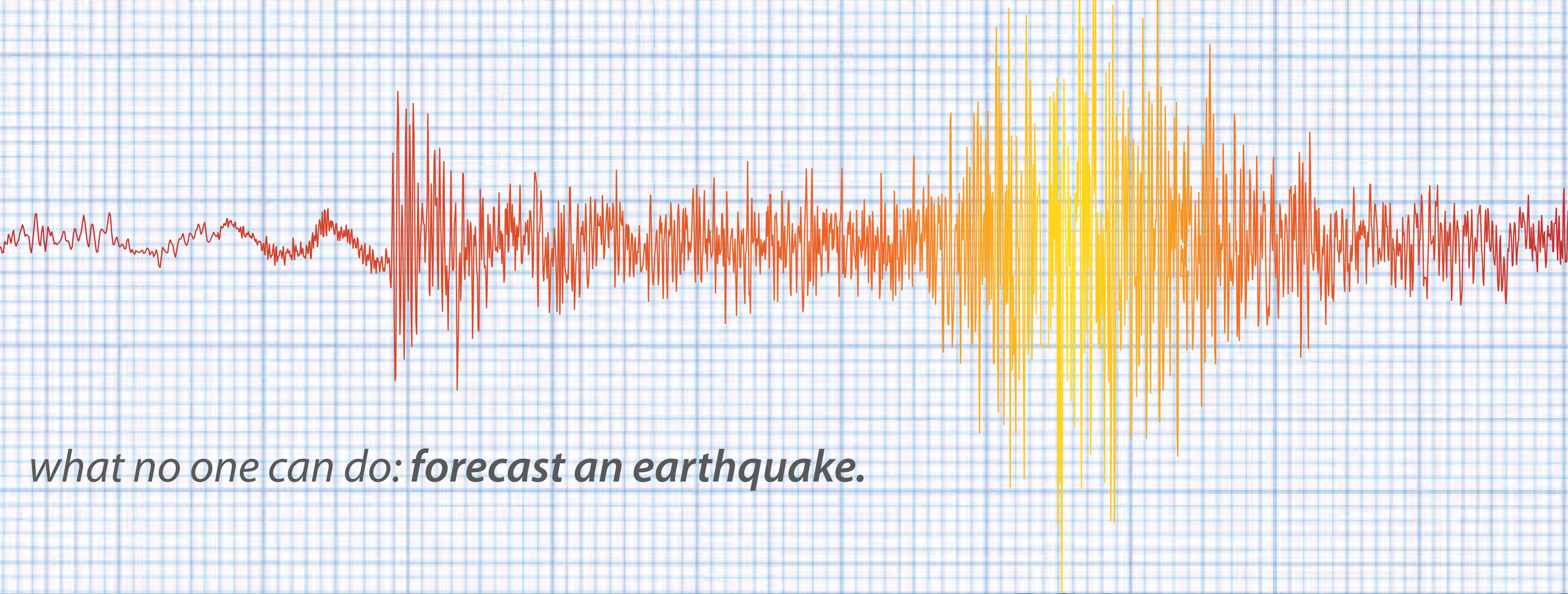
The prediction was the result of a combination of seismic rumblings (foreshocks), changes in well-water levels, and abnormal animal behavior. Based on these observations, state officials ordered a massive evacuation of Haicheng, and the next day a 7.3 magnitude earthquake shook the city, toppling empty buildings and filling empty streets with rubble and debris. The prediction was lauded as an extraordinary achievement, and shortly thereafter began the controversy. The methods failed to predict subsequent quakes and even 40 years later have yet to successfully predict another major earthquake.

Faulty faults

Earthquake scientists fall firmly into two camps: those who think all earthquakes are random events, caused by swirling thermal processes deep within the earth, and those who think that some quakes are actually triggered by others or are connected. Los Alamos geophysicist Paul Johnson is a member of the connected camp and believes that some earthquakes are triggered by seismic waves generated from far-off, previous earthquakes. He is studying what he describes as a modulating effect, in which earthquakes that eventually would have happened anyway (thermal swirling) actually happen sooner as a result of seismic perturbations from across the planet. By applying mathematical models and physical laboratory simulations, he and his collaborators want to understand how large earthquakes change the physical properties of the earth's crust and how these changes can lead to triggering of earthquakes in general—and temporal clustering of earthquakes in particular.

"Since the last turn of the century there have been about 15 really large earthquakes," Johnson says. "Are they all related?" He believes it's likely they are, and he's got the stats to back it.

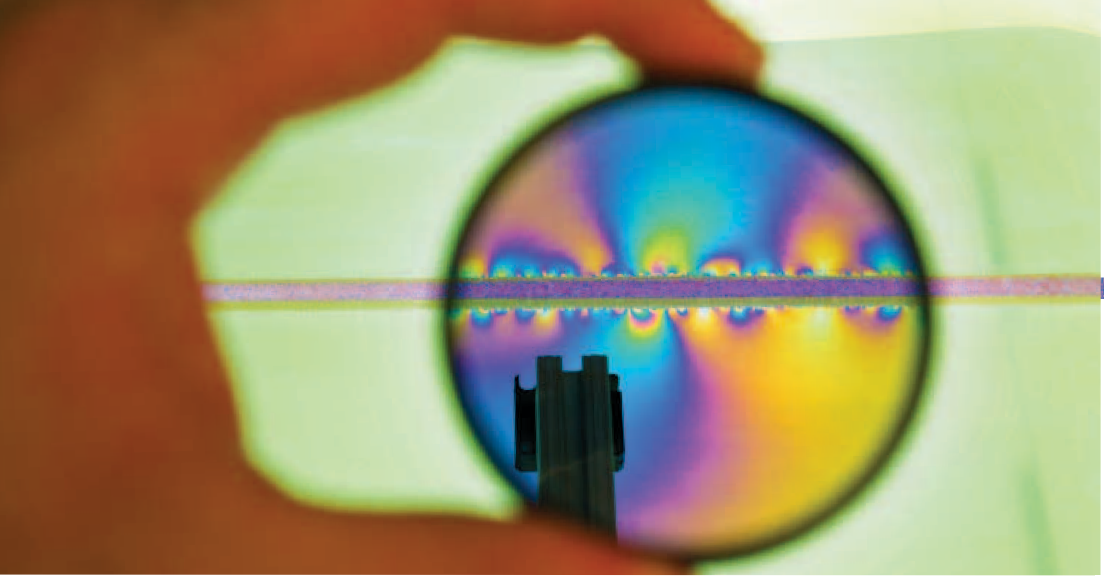
The surface of the earth, the watery and rocky layer within and upon which life exists, sits atop the deeper layers of crust and uppermost mantle, collectively referred to as the lithosphere. The earth's brittle lithosphere is broken into eight major tectonic plates (as well as myriad smaller ones), which are the basis of plate tectonic theory, the theory describing global geophysical processes such as continental drift and seafloor spreading. These plates are constantly moving and interacting, either sliding beneath one another in what is called subduction, or sliding past each other like opposing lanes of traffic in what is called lateral slipping. During these interactions, stress builds up along both sides of the fault (the interface of the two plates), and when the stress reaches a critical level, a slip event, or failure, occurs. If the failure is sudden, and the amount of built-up energy is large, an earthquake results.



what no one can do: ***forecast an earthquake.***

Johnson believes that seismic waves from large earthquakes temporarily decrease the elastic modulus of the weaker portions of the earth's crust—a measure of the ability of an object or material to resist stretching or compressing in response to being pulled apart or squeezed together. The decreased modulus, in effect a temporary softening of crustal material, extends over large distances, up to thousands of miles surrounding the fault, and preconditions additional faults within this range for accelerated failure. The extent to which the modulus is reduced and the time it takes to recover depend on both the strength and duration of the impinging seismic waves. As the perturbations generated from a very strong earthquake ripple through the land, toppling furniture and emptying cupboards, a similar degree of chaos occurs within the lithosphere. Small, medium, and large pieces of rock shift to energetically less stable configurations. Their unstable packing means they are in a state of increased interaction and decreased elastic modulus—thus perfectly charged to produce a quake.

Johnson and Los Alamos physicist Eli Ben-Naim, along with former postdoctoral researcher Eric Daub (now at the University of Memphis), have shown statistically that after a large quake, additional large quakes occur more frequently than a random pattern would predict. But the amount of data available from real earthquakes is severely limited because the seismic record only goes back about a hundred years and because data is only available after the fact, whereas the conditions *before* the quake are what are really important for establishing causation. To overcome these real-world limitations, Johnson's Los Alamos collaborators Scott Backhaus, Robert Ecke, and Drew Geller have



(Left) Viewed through a polarized camera lens, photo-elastic plates reveal discrete points of stress buildup along both sides of the modeled 2D fault as the far (upper) plate is moved laterally along the fault. (Right) The fault gouge is visible as tiny blue and red particles.

developed a 2D tabletop simulator that models the buildup and release of stress along an artificial fault. Using this experimental setup, they have compiled a virtual seismic record of quake events performed under precisely controlled conditions.

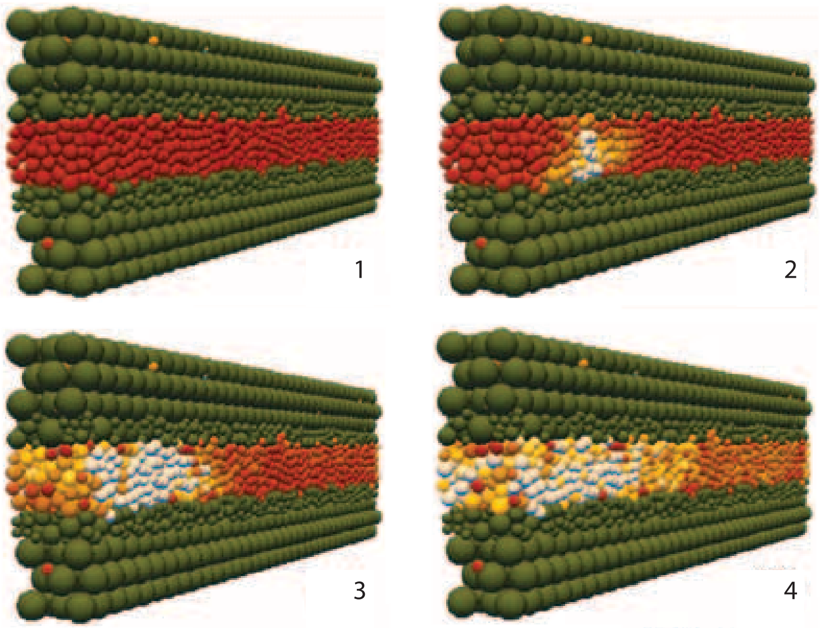
Therein lies the gouge

A key component of both natural and simulated faults is fault gouge. This is a vertical layer of granular material about 10–100 centimeters (cm) wide that fills the fault and is formed from the relentless grinding of tectonic plates against each other—like two sugar cubes being rubbed together, causing loose sugar granules to break free and accumulate. One of Johnson's major hypotheses is that fault gouge mediates the changes that lead to earthquake triggering. In the 2D experiments, the fault is 1 cm wide and 50 cm long, packed with small, vertically upright nylon cylinders (which would be spheres in a 3D system). Each cylinder is labeled with a tiny red dot or a tiny blue dot to indicate diameter (1.2 millimeters for blue, 1.6 millimeters for red)—this is the gouge.

During a simulation, the machine squeezes two horizontal "tectonic" plates of semi-rigid, plastic against each other laterally, with the gouge layer sandwiched in between them. Computer-controlled instrumentation applies a predefined amount of force to squeeze the plates together, compressing the gouge, and then slowly slides one plate laterally along the fault in a process called shearing that mimics the lateral slipping of real tectonic plates. The plates in the experiment also have tiny steel ball bearings glued to their upper surfaces adjacent to the gap. These detect the response of the semi-rigid plates to the forces of the gouge particles and also aid in measuring granular interactions and the size of quake events during experiments.

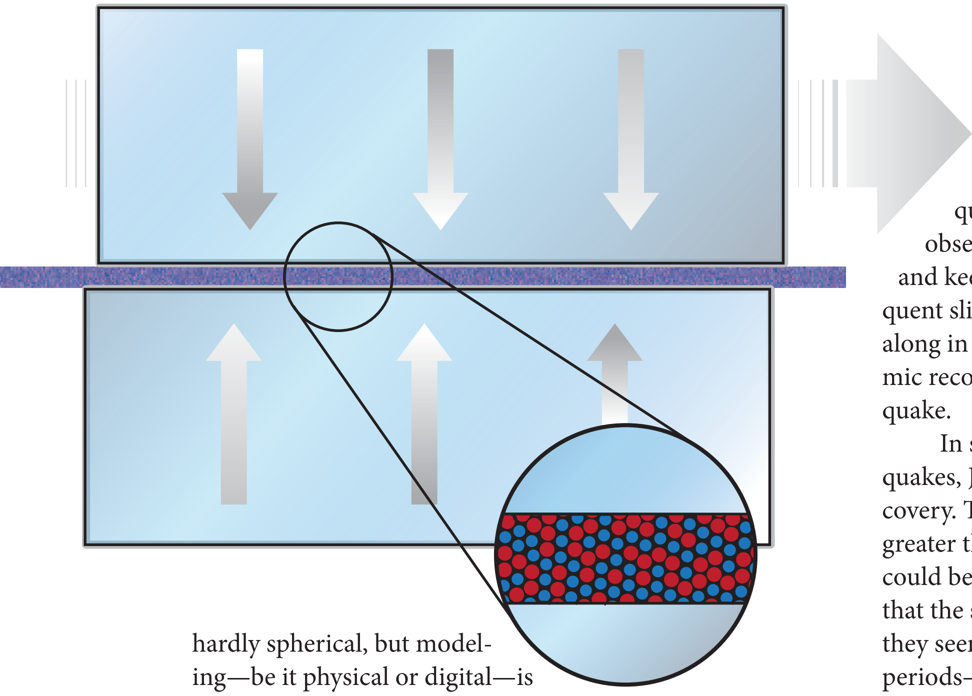
As the plates are sheared, the gouge is compressed and the particles rotate and shift, trying to find a more stable place to be, which in turn exerts pressure along both sides of the fault. The faster the plates are moving, the more pressure builds up; the more pressure builds up, the higher the elastic energy of the imminent failure. The whole apparatus is backlit so that cameras with polarizing lenses can capture images and videos of the shearing and slipping, and computers can determine the buildup and release of stress in terms of both magnitude and direction. This, then, tells the researchers where and by how much the elastic modulus is reduced, thus informing the forecast of future, triggered quakes within the same experimental setup.

To really understand how the gouge operates and participates in failure, the team uses 3D computer models in which the gouge is represented by spheres of various sizes. (True gouge particles are



Computer 3D modeling of gouge layer behavior during shearing. As the upper tectonic plate (top green layer) moves laterally with respect to the lower plate (bottom green layer) the movement of particles in the compressed granular layer (orange), is observed and measured. The lighter the color of the particle, the greater its speed. (1) No movement occurs during "stick phase," (2) localized movement occurs at the site of slip initiation, (3) as more gouge particles begin to move the slip spreads, and (4) extensive movement occurs in the granular layer as the slip propagates throughout the modeled fault.

CREDIT: Behrooz Ferdowsi, Jan Carmeliet, and Michele Griffa/ETH Zürich

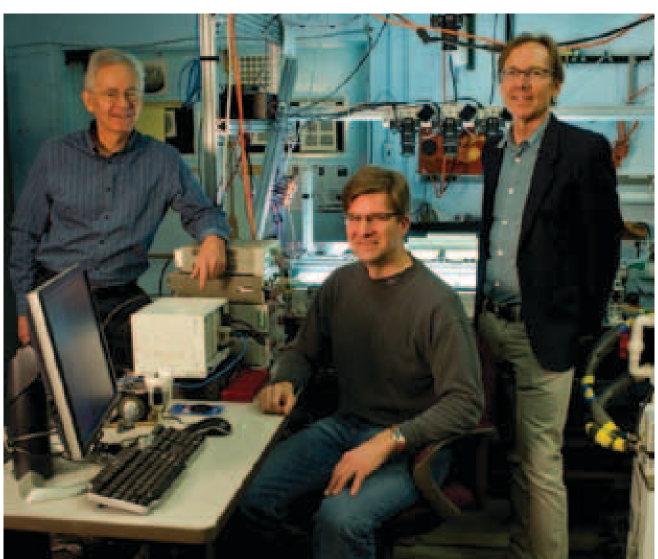


conditions correspond to either a spontaneous quake setup (no reduced modulus) or a triggered quake setup (reduced modulus), and the researchers observe how the gouge particles behave during shearing and keep records of the timing and magnitude of subsequent slips. Then, when the next large earthquake comes along in real life, they will compare it to this simulated seismic record to see if it looks like a spontaneous or triggered quake.

hardly spherical, but modeling—be it physical or digital—is all about approximation.) The computer models are used to develop templates, sets of conditions that reliably produce a particular result, which are then field-tested against real quakes. Data from a field site in Japan have recently shown that the models scale-up nicely. After the 2012 Indian Ocean earthquake, crustal disturbances exactly like those the templates predict were measured in Japan, approximately 2500 miles away. Just one other field site, this one closer to home (California), has the instrumentation required to test the templates; now it's just a matter of waiting—the researchers find themselves in the paradoxical position of rooting for a big one.

Trigger happy

Meanwhile, back in the lab, the experimental team has so far built a robust data set of spontaneous, isolated earthquakes that have been physically and digitally modeled. Now that they have determined how gouge behaves in a simple fault and what processes are associated with spontaneous earthquakes, the next step is to look at dynamic earthquake triggering—that is, when one earthquake induces another by setting the stage via less-stable packing. To simulate reduced elastic modulus of the earth's crust, as would be seen after a large earthquake, the force applied to the gouge from the plates in the 2D experiment is minutely increased. The input



In studying the historical record of very large earthquakes, Johnson and Ben-Naim made an interesting discovery. They looked at all great earthquakes (magnitude greater than 7.5) since 1900 and, after removing quakes that could be confirmed to be aftershocks of other quakes, found that the strongest quakes did not occur randomly. Rather, they seemed to be temporally clustered in two distinct time periods—mid-twentieth-century and the present. In other words, we may be currently in the midst of a connected series of triggered earthquakes. This is potentially bad news for humanity, but great news for science. But because the sample size is small, the statistical support is weak. However, with each new large quake the sample size grows by one, and comparison to Johnson's virtual seismic record becomes that much better at telling how accurate his team's models are—which, so far, is very.

In addition to modeling triggered earthquakes, the team would like to increase the complexity of their fault to better model a natural fault. What influence, for example, does the presence of groundwater in the fault have? Or what about a nonlinear fault with variable width? What about making the gouge more complex in terms of composition and particle size? It's no small feat to build a good laboratory fault experiment, and building one that can incorporate all these variables is still a ways off. So for now, 2D tabletop experiments and 3D computer modeling are where it's at—still leaps and bounds better than observing animal behavior and well-water levels.

This is the challenging reality of earthquake prediction. As Johnson says, "Forecasting is as good as it gets. It's doubtful we'll ever be able to truly *predict* earthquakes." But if he's right about triggering, and one good crack brings about another, then the theory of plate tectonics needs to be re-examined—specifically, the strong modulating influence of earthquake interaction. And there's a practical application as well, in hazard assessment and mitigation. Like the proverbial bad apple, one bad earthquake spoils the landscape for a whole bunch more—but knowing how quickly, how far, and for how long the bad apple's effects can spread may help to ease its bite. LDRD

—Eleanor Hutterer

Los Alamos scientists (left to right) Robert Ecke, Drew Geller, and Paul Johnson in front of their 2D tabletop experiment. By studying the interactions of granules within the fault, they are learning how earthquakes alter the earth's crust, preconditioning it for additional quakes.

Body Building

Stable isotopes reveal biodiversity in the manakin diet that may be key to their future survival

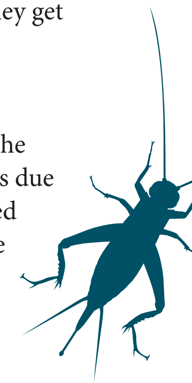
A QUICK GLANCE AT SOMEONE ELSE'S SHOPPING CART AT THE GROCERY STORE can convey a great deal about a person's diet. All health judgments aside, a vegetarian may have veggies, tofu, and nuts; while an omnivore might skip the tofu and add a steak. A pregnant mom may be loading up on protein, a young athlete piling on carbs, and an elderly shopper buying less food altogether. Humans and animals don't always have the luxury of choice when it comes to their diets, but when they do, it can be illuminating to see what they choose. Because you are what you eat, these choices impact the detailed composition of your body.

But it's not just about choice. Food selection for many animals is more about survival than personal preference; if a species relies too heavily on one food source, and that food becomes threatened by environmental changes or disease, the species may become threatened as well. Dietary habits may also play an important role in an ecosystem, such as by dispersing seeds or cleaning up debris. Variety in diet can translate into a better chance for survival for that species as well as those dependent upon it in the food chain.

Since scientists can't ask animals about their diets, they instead have to rely on observations of animal behavior, coupled with analysis of animal excrement, to determine what the subjects have eaten. This method is fairly reliable, but also limited because fecal samples are only representative of what was consumed recently.

Gaining popularity as an indicator of diet is the analysis of stable (nonradioactive) carbon and nitrogen isotopes assimilated into animal tissue. In all organisms, some food is consumed for energy, and some is broken down and used as building blocks for new growth. Stable isotopes help uncover clues about the latter. Scientists at Los Alamos recently applied their expertise in stable isotopes to analyze bird feathers from Ecuadorian manakins, small, fruit-loving birds who distribute seeds in their Amazon habitat—a key ecosystem service. Using a specialized algorithm developed to incorporate uncertainty in the isotopic concentrations from

each food source, the scientists were able to thoroughly examine the diet of the birds and the destination of the atoms they get from their food.



You are what your food ate

Hidden between the lines of the periodic table are the isotopes—different versions of the same element, each with a slightly different mass due to their nuclei having additional or missing neutrons. For decades, scientists have measured and exploited the decay rate of unstable isotopes. For example, carbon-dating of materials is done by examining the ratio of stable ^{12}C (read "carbon-12") to unstable ^{14}C, which has a half-life of nearly 6000 years. Some stable isotopes—especially relatively rare isotopes of life-sustaining elements such as carbon, hydrogen, oxygen, or nitrogen—are also useful in biological research as they vary predictably by geographic region and can be used as signatures of an organism's lifestyle.

For instance, rainwater—and therefore drinking water—in coastal areas is enriched with more of the isotope oxygen-18 than that from inland areas and higher elevations. This is because raindrops containing ^{18}O tend to precipitate first, before the much more common ^{16}O, and as rainstorms move inland from the coast, fewer ^{18}O water molecules remain in the cloud, in comparison to ^{16}O and ^{17}O. (All three isotopes are stable, and the differences are miniscule but measurable.)

Plants are often characterized by their specific method of converting carbon dioxide (CO_2) to sugar and other carbohydrates—a process called carbon fixing. So-called "C_4 plants" include corn and sugar cane, and the more common C_3 plants include rice and wheat. Because of a difference in the enzyme used in C_4 plants, they accumulate slightly more ^{13}C. As a result, people in North America who eat more corn (or corn-fed beef) have a higher ^{13}C isotope profile.

"You can measure differences in isotopic composition that exist along a human hair that may indicate that a person has moved from one [geographic] region to another, based on the isotopes assimilated from their diet," explains Dave Podlesak, a chemist who is involved with a number of stable isotopes projects at Los Alamos. He says that for years forensic scientists have been evaluating stable isotopes in hair and fingernails, which are constantly growing and incorporating new atoms, thereby keeping a record of the available isotopes.

Forensic scientists must keep in mind that an organism's isotope profile comes primarily from the food and water consumed but also can be impacted by its trophic level, or place in the food chain. With nitrogen, for example, organisms tend to preferentially excrete ^{14}N (the most abundant form of nitrogen) and accumulate ^{15}N because the lighter isotope reacts slightly faster due to lower bond strength and is, therefore, excreted before heavier ones, which are often assimilated. When one organism eats another, the ^{15}N accumulation is compounded. In the same manner that a high-level predator such as a tuna fish can have a greater concentration of mercury than other animals by accumulating it from many trophic levels of its prey, an organism cumulatively gathers isotopically heavier nitrogen from its food sources as well.

"In general, each trophic level enriches the ratio of ^{15}N to ^{14}N by about 3 per mille [parts per thousand]," says Jeanne Fair, a biologist who led the Los Alamos portion of the manakin research.

Sticky situation

The Amazon rainforest is one of the most biologically diverse places on the planet. It is home to hundreds of bird species, many of which are crucial for ecosystem function, as they disperse seeds and nutrients, pollinate flowers, eat pests, and scavenge on forest debris. These ecosystem services, in turn, are critical for the health of the forest; the plants that grow as a result of the birds' seed dispersal are food for other animals, and those animals may be food for larger predators. The rapid loss of tropical birds due to climate or environmental changes may significantly disrupt their ecosystems.

For the last ten years, the National Science Foundation (NSF) has funded a multi-institutional study of manakin birds in their habitat in the Amazon. The studies have been done at the Tiputini Biodiversity Station, in the Yasuni Biosphere Reserve in Ecuador. The Reserve is a haven of biodiversity and is home to nearly 600 bird species and more than 100,000 different species of insects, not to mention amphibians or mammals. The Reserve also happens to be located atop an estimated hundreds of millions of barrels of crude oil, making conservation of the rainforest the subject of heated debate. In fact, in 2007, Ecuadorian President Rafeal Correa offered to protect a significant sub-section of the drilling area in hopes that the global community would contribute funds to his country in lieu of the oil revenue Ecuador would be giving up (as gratitude for the green gesture). But he abandoned the idea in 2013 after only $13.3 million had been received out of $300 million pledged—both far less than the $3.6 billion he had hoped for.

Because of their role in seed dispersal, manakins are very important to the welfare of the Amazon forest. The researchers in the NSF study, who are from the University of Florida, Gainsville, and the Smithsonian Migratory Bird Center in Washington, D.C., hope to find out more about them before the drilling permanently changes their ecosystem.

"If you take the manakins or other seed-dispersing species out of the forest, the forest will change, and we have no idea how to predict those changes," says Fair.

One aspect of their investigation has been to study the diet of six species of manakins that live closely together in the area near the Tiputini station. Among the advantages of studying manakins is that they are neither migratory nor live in a particularly unstable environment (yet), both of which can alter stable isotope assimilation. Understanding more about their diet could help the team evaluate their vulnerability in the changing Amazon.

The diet analysis took place over a period of two years, during which the team captured and examined 147 individual birds representing all of the six species. Upon capture, a small length (2–3 millimeters) of the tip of the middle tail feather was clipped for stable isotope analysis; fecal samples were routinely collected as well. The scientists also observed the birds foraging and took samples of what they were eating: plants with ripe fruit and insects such as crickets, ants, and larvae. It was previously known that frugivorous (fruit-eating) birds often complement their diet with insects to obtain protein. The investigators hoped the stable isotope analysis at Los Alamos would help quantify how much of the manakins' diet is actually made up of insects.

Early bird catches the…

In order to understand the manakin diet, the team analyzed both the assimilated ^{15}N and ^{13}C in the bird feathers and the isotope ratios present in each food source. First, the team dried and homogenized the feathers, fruits, and insect samples before they were fed into an analyzer, which burned and purified the organic matter into CO_2 and N_2. Finally, a mass spectrometer ionized the gases and separated the isotopes for quantification.

"It would have been very easy to look at these absolute data [on isotopic concentration] and see that they didn't correlate with the fecal and foraging data, but we wanted to be more thorough and decided to add the mixing model approach," explains Jeff Heikoop, a geochemist who, along with colleague George Perkins, completed the isotopic analysis at Los Alamos. Heikoop and Perkins decided to use an isotopic mass-mixing model, which they had previously used in another project evaluating river water for evidence of nuclear processing. Los Alamos sub-contractor Paul Davis developed the algorithm.

"We used this mixing model to look at the isotope profile of rivers for the Global Security program at Los Alamos,"

Sample	δ^{13}C ‰	δ^{15}N ‰
	-32.1	1.3
	-25.0	3.7
	-27.8	4.0
	-33.0	5.8

Each component of the manakin diet was measured for its individual stable isotope profile. As is standard in all stable isotope research, the raw numbers are given context by comparison to an accepted calibration protocol: atmospheric nitrogen for nitrogen, and a specific fossil carbonate for carbon. For example, a measurement of ^{15}N/^{14}N in a larvae is written δ^{15}N= 5.8 ‰ indicating the larvae has a measurement of 5.8 parts per thousand more ^{15}N/^{14}N than the ratio of the same nitrogen isotopes in the atmosphere. The profiles of the food sources were then compared to the profiles of feather clippings from all the captured birds.

says Julianna Fessenden-Rahn, a chemist in the Defense Security Analysis Division, who led that project. "We tried to find signatures of nuclear processing hidden among isotopes from other sources such as fertilizer effluents." For both the river analysis and the manakin study, the challenge was to identify the ranges of values from each source and how they could mix or change in the system being analyzed (a river or a bird).

The manakin research team corrected for the trophic level isotope effect for fruit and insects before using the data in the mixing model. Next, the algorithm incorporated the effects of isotopic uncertainty from the food sources in a way other models would not have allowed. "We were able to look at two isotope systems in each feather sample, $^{15}N/^{14}N$ and $^{13}C/^{12}C$, and find dietary mixing solutions consistent with both," says Heikoop.

In the end, the model gave them 5.9 million possible combinations of fruit and insects that could match the isotope ratios found in the feathers. The results broadly indicated a greater percentage of assimilated ^{15}N coming from insects as the food source. This supported the notion that the manakins are not completely frugivorous and that they eat a significant amount of insects to obtain more protein.

Nitrogen is a key component of amino acids, the building blocks of protein, and protein is a major component of feathers. With this in mind, the team's data might underestimate the amount of fruit in the manakin diet because it may have been mostly used for energy, instead of for making feathers. The researchers also realized the birds must get a large proportion of nitrogen from larvae, spiders, and other soft-bodied arthropods that do not leave indigestible exoskeleton remains in their feces and are, therefore, missing in the fecal analysis. When the stable isotope data were combined with the observational and fecal data, the team was able to construct a comprehensive picture of the manakin diet and the assimilation of nutrients into their feathers.

A *Pipra filicauda* manakin in Ecuador's Yasuni Biosphere Reserve

So they're not herbivores

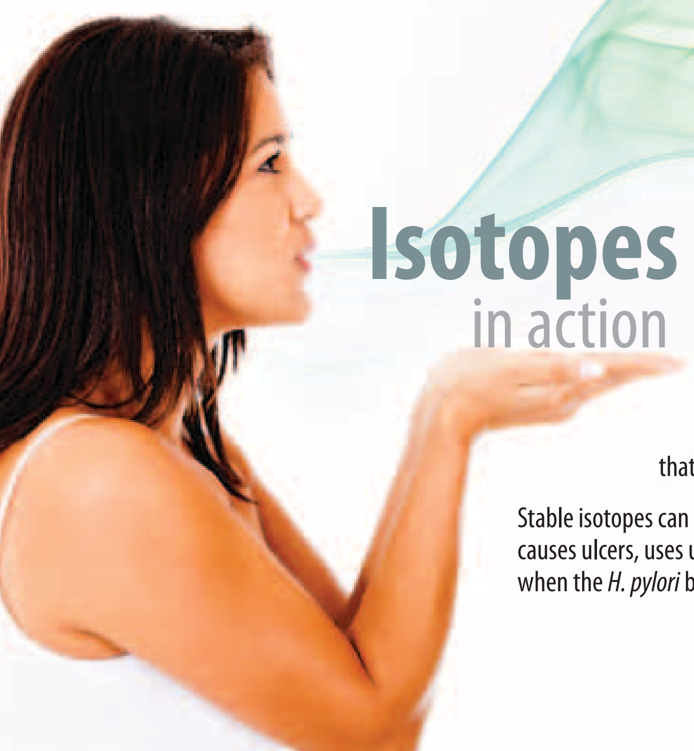
Confirmation that manakins do indeed consume insects is a valuable data point towards understanding their fate in a changing ecosystem.

"Some of the questions we as researchers ask are, 'What is going to drive adaptability to climate change?' and 'Are these species capable of rapid evolution?'" says Fair.

Since the manakins vary their diet, they may be less vulnerable to extinction if their surrounding environment is altered—which is good news, considering their important role in the forest. Other species, however, may not be as adaptable, and Fair explains that, if identified, those more fragile species could become the recipients of focused conservation efforts. While the whole goal is to preserve as much biodiversity as possible, species that provide critical ecosystem services may be especially important—not just to a particular ecosystem, but to humanity as well.

"Biodiversity is the best predictor of resilience and adaptability," says Fair. "The fundamental truth is that biodiversity matters profoundly to human health in almost every conceivable way. The roles that species and ecosystems play in providing food, fuel, and unique medicinal compounds; the purification services for air, water, and soil; and the natural regulation of infectious disease, to name a few, are critical to our health and survival."

—Rebecca McDonald



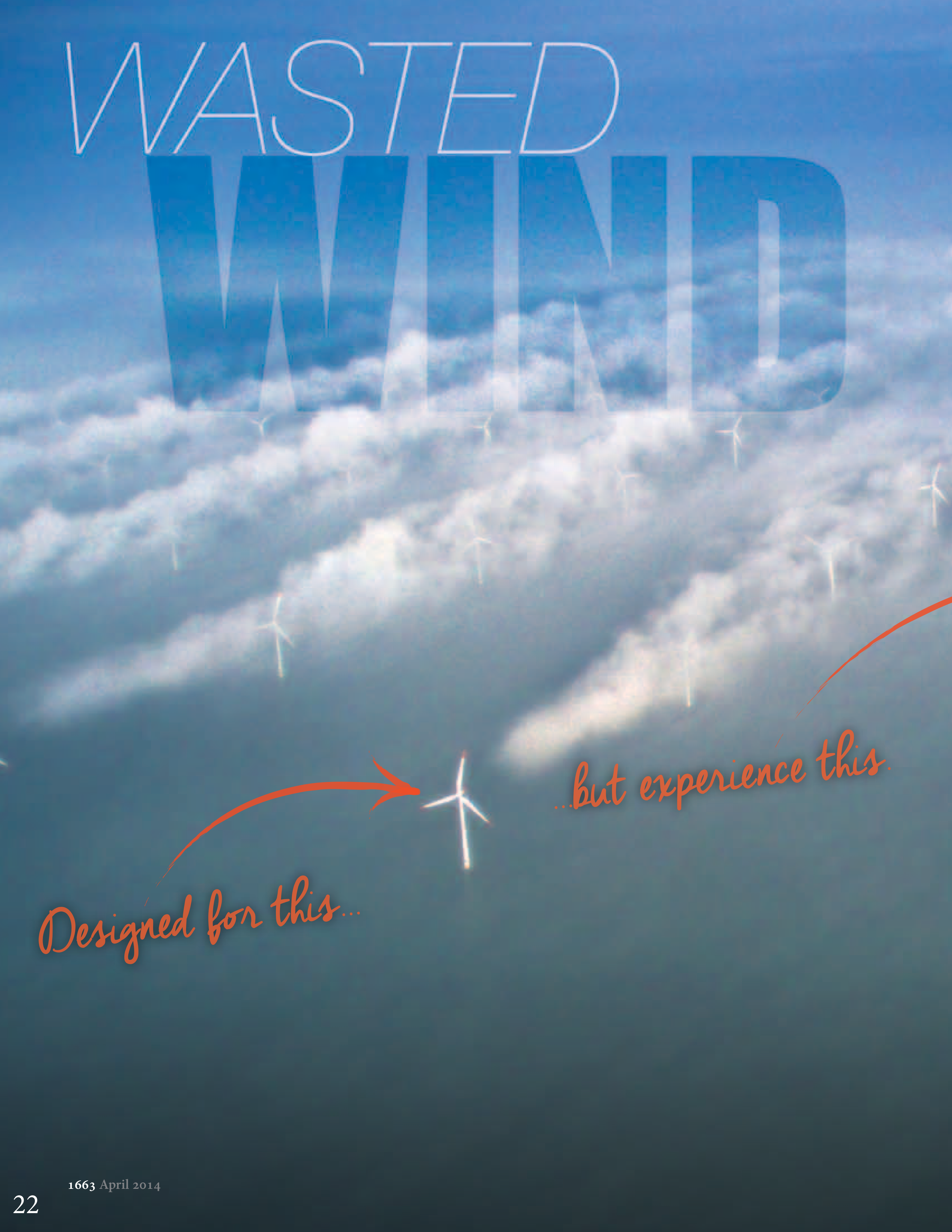
Isotopes in action

Stable isotopes have been a part of research at Los Alamos for nearly five decades. In the 1960s, scientists at the Lab were the first to create and automate large-scale separation of ^{13}C from ^{12}C. This enabled researchers to introduce stable isotopes to a system as tracer molecules or labels in research, as opposed to measuring stable isotopes that naturally exist in an organism.

"Stable-isotope labeling is valuable for evaluating chemical and biochemical reactions and for analyzing metabolites, proteins, and other biomolecules," says Los Alamos biochemist Cliff Unkefer. When possible, stable isotopes are useful in place of radioisotopes that may have adverse effects on the study.

Stable isotopes can also be used in medical tests. The diagnostic test for *Helicobacter pylori*, the bacterium that causes ulcers, uses urea labeled with ^{13}C as a tracer. Patients swallow the tracer (dissolved in orange juice) and when the *H. pylori* break down the urea into ammonia and CO_2, the ^{13}C can be detected in the patient's breath.

WASTED WIND



"WHY AREN'T THEY TURNING?"

It's a windy day, and even though some of the wind farm's turbines appear to be turning as they were designed to, many are barely turning, and several aren't turning at all. It looks as though a lot of energy is going to waste.

Indeed, each of the massive, state-of-the-art turbines is designed to extract several megawatts (MW) of energy from the wind, with the largest capable of generating 7.5 MW. That's enough power from one turbine to provide for more than 700 average Americans on an ongoing basis, and 100 such turbines would out-produce some nuclear power plants. Yet these wind turbines routinely underperform their predicted power output and suffer mechanical failures that prevent them from turning at all. According to the U.S. National Renewable Energy Laboratory, wind farms typically perform at 10 percent below expectations—and sometimes as much as 40 percent below.

Meanwhile, the demand for wind power to reduce humanity's reliance on fossil fuels continues to grow. And in a way, that's part of the problem. Because as the demand has grown, so too have the turbines themselves. This was not unexpected, since the power they collect is proportional to the area of the circle swept out by their blades. Bigger should mean better. But great size brings unexpected vulnerabilities.

"Unfortunately, the growth of wind turbines has outpaced power companies' knowledge of their dynamics within wind farms," says Curtt Ammerman, the head of a Los Alamos research team striving to make wind turbines more effective.

Size isn't everything

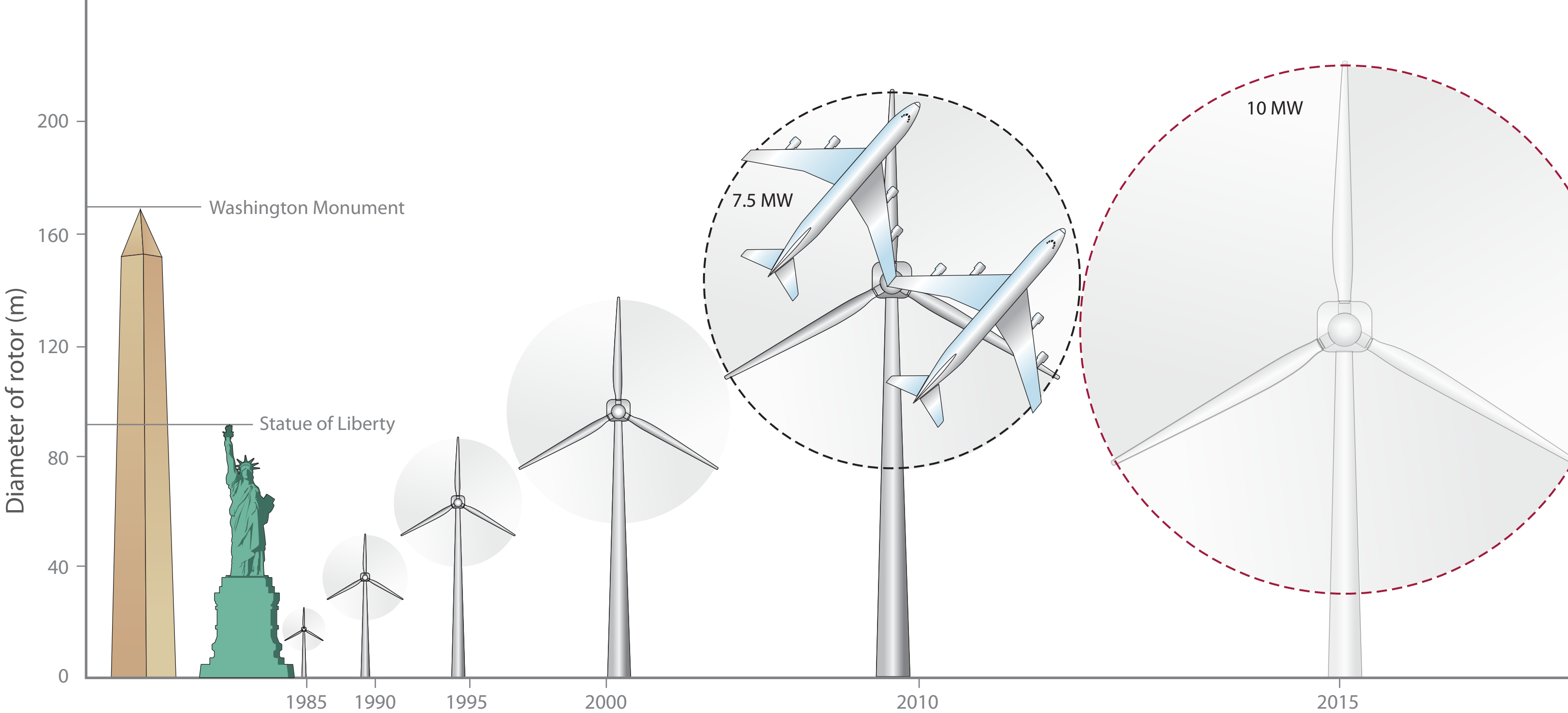
The largest wind turbines in operation today stand on towers 135 meters (m) tall and have rotating assemblies, or rotors, 126 m in diameter (including the blades). To put that in perspective, the wingspan of a Boeing 747 jumbo jet—similar to the one the U.S. president flies around in—is only 64 m, or about half the diameter of the turbine rotor. The diameter of a wind turbine from the early 1980s was about one-tenth of what it is now. And rotors continue to grow even bigger: a 10-MW offshore model with a whopping 190-m rotor diameter is currently under development.

What's the problem with such a large-diameter wind turbine? Standing by itself in a perfectly smooth flow of wind, nothing. But in a turbulent flow, whether that turbulence is caused by the weather or by the wake from another large turbine positioned upstream, a large diameter can become a liability. Any differential force applied near the ends of such long turbine blades can produce severe bending stresses in the blades and a tremendously amplified torque at the center, where the system's gearbox and electrical generator reside.

"These big, beautiful, modern wind turbines have a design life of 20 years and yet break down, on average, two or three times in the first 10 years," says Ammerman.

This aerial photo of Denmark's Horns Rev 1 offshore wind farm was captured just as weather conditions created fog in the wake of each wind turbine. The more turbulent downstream air can cause power losses and mechanical problems for turbines behind the front row.

CREDIT: Christian Steiness/Vattenfall



Wind turbines have grown rapidly in the past two decades in order to meet the rising demand for renewable energy. But with larger sizes come not only more power, but also larger torques, more frequent damage to the central hub, and higher repair costs.

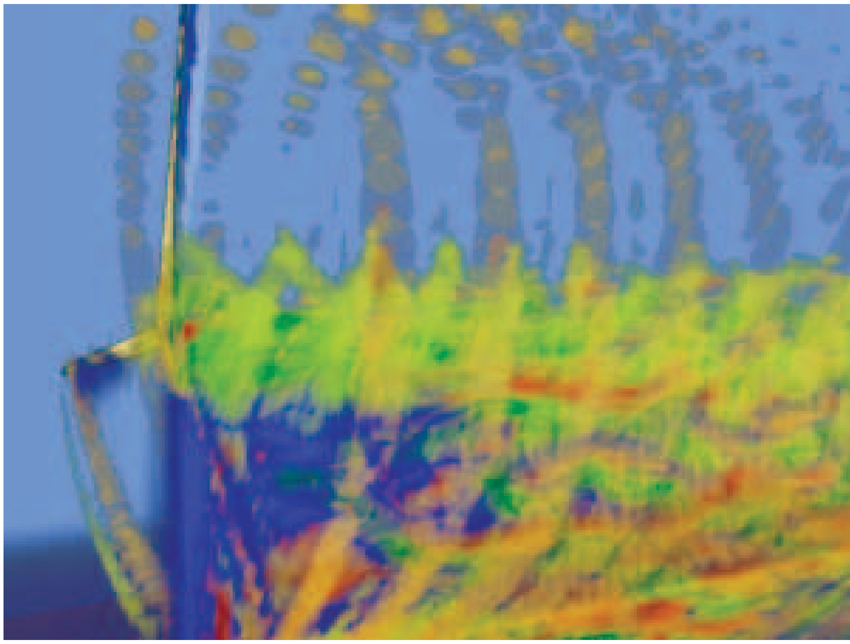
Not surprisingly, most of the downtime-causing damage suffered by wind turbines in the field afflicts their gearboxes (60 percent), generators (14 percent), and rotor blades (7 percent). Just as a long-handled wrench makes it easy to turn a nut, a long-blade turbine makes it easy for turbulent wind to monkey with the gearbox and generator—which is partly why it's so common to see wind turbines that aren't spinning. (Other times, the arrangement of turbines and the path of the wind can combine to produce temporary dead spots in the airflow.) Long turbine blades and correspondingly large diameters provide a great deal of leverage, which, of course, is desirable when it is applied to turn the rotor as intended. But when a turbulent wind stream twists the rotor out of its plane of rotation, then leverage can turn into damage.

To make matters worse, it's no simple matter to repair a damaged gearbox behind the central hub of a turbine rotor when it's one-and-a-half football fields off the ground. According to Ammerman, it's not unusual for it to cost more than a quarter-million dollars just to get a crane large enough to reach the hub of a damaged turbine out to the site; the cost to repair or replace the broken component comes on top of that.

"That's why you'll often see multiple turbines not spinning, instead of just one," he says. "They're so expensive to repair that it's more economical to wait until a number of them are broken before getting a crane to fix them all at once."

Bumpy ride

Rod Linn and Eunmo Koo are atmospheric modelers on Ammerman's team. They figured out a way to repurpose a supercomputer-based simulation tool originally designed to model the evolution of wildfires into one that analyzes the interaction between spinning turbines and the wind around them. Within this numerical simulation, called WindBlade, it is possible to vary any number of parameters to obtain realistic results, including the turbines' power output and the forces on the blades—and therefore the torques delivered to the hub as well. A wide range of scenarios can be tested,



The turbulence in the wake of a modern wind turbine is predicted by the Laboratory's WindBlade supercomputer simulation.

including wind flow that's uneven, gusty, turbulent, or shifting around in direction.

The parameters of the wind farm can be adjusted as well by varying the size, number, and arrangement of its turbines. In addition, the turbines can occupy a variety of landscapes by introducing hills and even heterogeneous vegetation. (Such complex supercomputer modeling is a major component of what Los Alamos brings to the table in wind energy and other research.)

The simulation results were eye-opening. They showed, for example, that a large wind turbine positioned somewhere behind the front row in a wind farm would experience stresses that varied wildly—not just in time, but also from one blade to another, and even from one part of a blade to another. These stresses would shift about quickly, growing and shrinking by nearly a factor of 10 over a period of seconds. Harmful vibrations in the turbine blades and sharp jolts on the central gearboxes were commonplace.

"I remember being taken aback by how much the mechanical stresses could fluctuate between the turbine blades from one moment to the next," Linn says. "And nobody had developed a thorough understanding of the nature of these loads or the turbulence that causes them, especially in a wind turbine array where numerous turbines are impacting each other."

Perhaps if the wind-power community had that understanding all along, they might have thought twice about meeting the ever-larger energy demand with ever-larger turbines. Or perhaps larger turbines would have proved to be the best option regardless. But even in that case, results from high-performance computing simulations like WindBlade could help engineers to make their designs more robust—or at least set their performance expectations more in line with the reality of turbulent airflows.

Large-diameter turbine rotors chew up the airflow for any other turbines located downstream. WindBlade revealed that after a 15-meter-per-second (m/s) wind passes through a 5-MW turbine, the wind speed immediately drops to about 10 m/s. It slowly regains speed as it flows downstream due to the entrainment of the surrounding wind (wind that didn't pass through the rotor) mixing in with it. But this return to the initial wind speed doesn't happen until well after 14 rotor-diameter-lengths downstream. That is, for a 100-m diameter rotor, the wind wouldn't recover to its original speed until a distant 1.4 kilometers behind the first turbine.

Of course, in the real world, not many wind farms can space their turbines kilometers apart. Often the spacing is more like seven rotor diameters and sometimes as close as three. WindBlade simulated of a series of 5-MW turbines,

The largest wind turbine in use today is 135 meters tall at the hub and 126 meters in rotor diameter.

one behind the next at a variety of spacing intervals to examine the sensitivity of power output to spacing. In one simulation with three-diameter spacing, the five turbines were exposed to a 15-m/s headwind (at hub height). The second turbine saw wind at about 10 m/s, as expected, but the third got only about 7 m/s—a huge drop from the initial 15 m/s. Then the wind speed rose a bit, leveling off for the subsequent turbines at around 8 m/s, as more wind from above the turbines mixed in, due to a combination of ambient and turbine-induced turbulence.

Best foot forward—or not

Why does the wind speed matter? Because in the theory of wind energy, the power a wind turbine produces is proportional to the wind speed cubed. If the wind speed gets cut in half—from the first turbine in Linn's simulation to the third, fourth, and fifth, for example—the power drops to a factor of one-half cubed, or one-eighth, of its full-speed level. In reality, the situation is more complex, and there isn't just a single, uniform wind speed approaching a rotor 100 or more meters in diameter. Regardless, a substantial power loss remains. For the simulation of five turbines staggered at three rotor diameters apart, the total power produced was only around 15 MW, not the 25 MW one might expect from five 5-MW turbines.

The team then repeated the previous experiment but changed one thing: they restricted the first turbine to 4 MW and kept the others at 5 MW. In real life, this could be accomplished from the control room; operators can adjust the pitch of the turbine blades (twist them) to extract less power and suffer less mechanical stress. Interestingly, they found that the combined power from all the turbines was actually greater as a result of the power restriction. This demonstrates the possibility of optimizing a wind farm and even reducing its original installation cost by placing smaller wind turbines in forward positions and regularly varying the blade pitch on different turbines to maximize the power generated by the farm overall as wind conditions change.

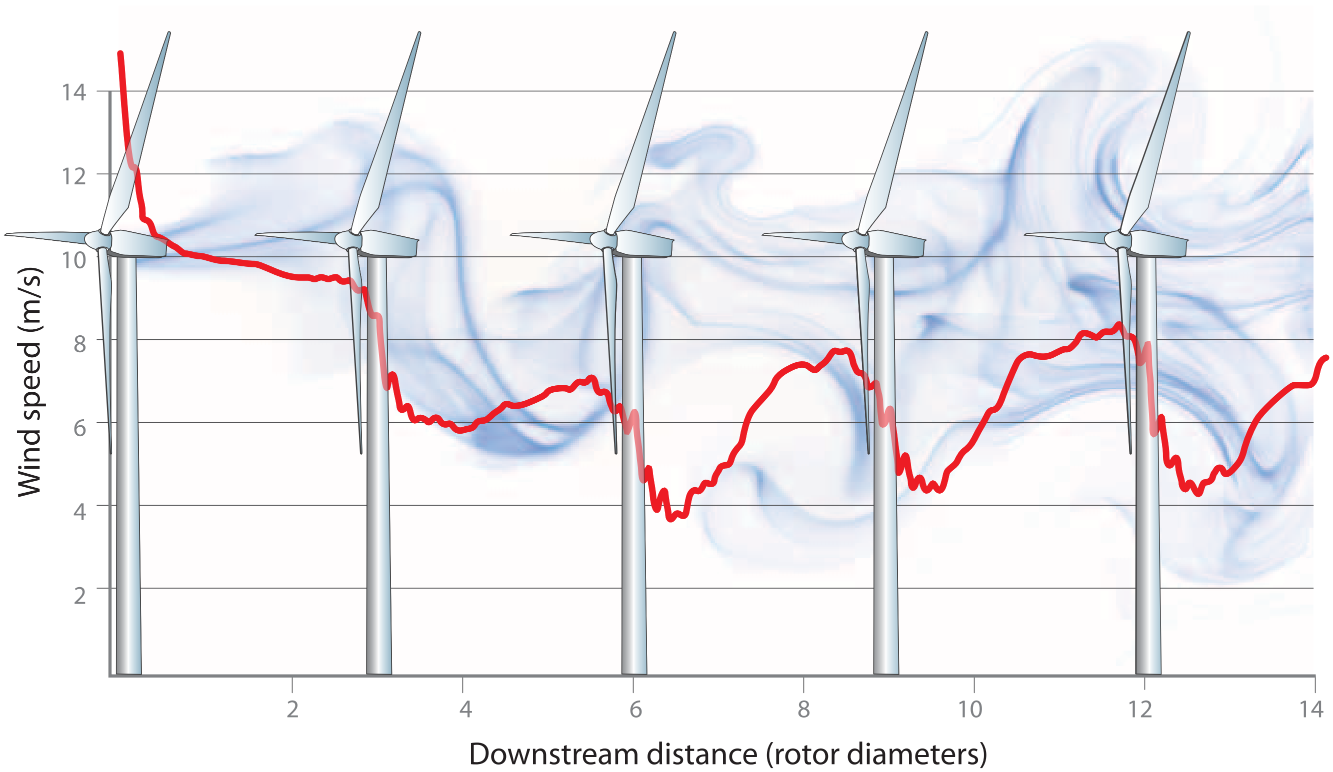
"That's where we want to go next," Linn says. "We want to provide tools and understanding that can improve the performance of existing wind farms, enhance the design of future wind farms, and supply new operational software to help the utilities run their wind farms at peak performance with minimal damage."

Such future software could tell operators when and how much to adjust the blade pitch on each turbine, moment by moment, to increase the power produced by the farm as a whole. It could also compute detailed stresses and torques and instruct operators to take action to prevent excessive damage accumulation on individual turbines under certain conditions. In fact, many of these improvements could be automated, with adjustments being made whenever various sensing systems detect changing wind patterns or mechanical stresses.

The Department of Energy (DOE) has set ambitious goals for wind power and will need advances like these to get there. It seeks to increase wind energy from a current 4 percent to 20 percent of the nation's total electrical consumption by 2030. The goal appears to be achievable; Iowa, South Dakota, and Kansas already obtain more than 20 percent of their electricity from wind. But even the comparatively paltry 4 percent for the nation as a whole has been achieved with a dramatic expansion of wind power installations in recent years. Getting to 20 percent nationally will require a continued increase in wind power installations to be sure, and it will also require improving wind farms' output-to-cost ratio, particularly by reducing turbine downtime. Otherwise, turbine repairs will remain too frequent and too expensive for wind energy to adequately displace fossil fuels.

"The DOE's 20 percent plan is an important one, at the same time reducing our carbon footprint and our reliance on foreign fuels, for better energy security," says Ammerman. "Fortunately, most of the turbine failures that currently hold us back from meeting that goal take place in the gearbox, generator, and blades—the same components our research can help to protect." LDRD

—Craig Tyler



Five simulated 5-MW turbines in a row, spaced three turbine diameters apart, produces a rapid loss of incoming wind speed that eventually levels off with about half of the initial wind speed reaching the turbines in back.

spotlights

Organic Light

About 15 percent of the average American household's electricity goes to lighting—and existing lighting technologies are notoriously inefficient. Even today's green-tech compact fluorescent bulbs and LED lamps convert only 8–14 percent of the electricity they consume into light. Nonetheless, that's still many times better than incandescent bulbs, which are only 2–3 percent efficient. According to the U.S. Department of Energy, rapid adoption of existing LED lighting over the next 20 years could save the country $265 billion and eliminate the need for 40 new power plants. Better yet, in theory, future LED lamps could operate at a staggering 40-percent efficiency or slightly more, blowing away everything that exists today.

Los Alamos materials scientist Sergei Tretiak, working with colleagues at the University of Utah and Nanjing University in China, recently made important headway toward that tantalizing 40 percent. The team experiments with organic LEDs, or OLEDs, made from organic-polymer semiconductors instead of traditional semiconductors like silicon. They have a flexible, plastic appearance and are currently used in computer, smartphone, and high-end television displays. In these applications, red, green, and blue fluorescing OLEDs combine to make each pixel. The same can be done to make white light for OLED lamps (as is currently done for LED lamps), but this approach is prohibitively expensive. Instead, the objective for OLED lighting, if it is to reach that approximately 40-percent theoretical limit, would entail individual white pixels doubling up on output by combining fluorescence with phosphorescence.

"Phosphorescence normally won't happen," Tretiak says, "unless you provide certain metals that enable crossings between fluorescing and phosphorescing states." He and his collaborators selected atoms of platinum and inserted them at particular intervals along the chainlike OLED polymer molecules. When inserted at every chain link, the polymer produced violet fluorescence and yellow phosphorescence; at every third chain link, it produced blue fluorescence and orange phosphorescence. Both mixtures appeared whitish, and the team demonstrated that truly white light should be possible after a little tinkering with more complex platinum spacing, to adjust the colors and their relative intensities.

Does that mean the OLED-lighting revolution is already upon us? "Not just yet," admits Tretiak. The team's experiments used an additional light source to deliver energy to the polymers, but a true OLED would supply the energy with electricity instead. "So there's another step to go," says Tretiak. "But producing multiple colors from a single polymer gets us much closer." LDRD

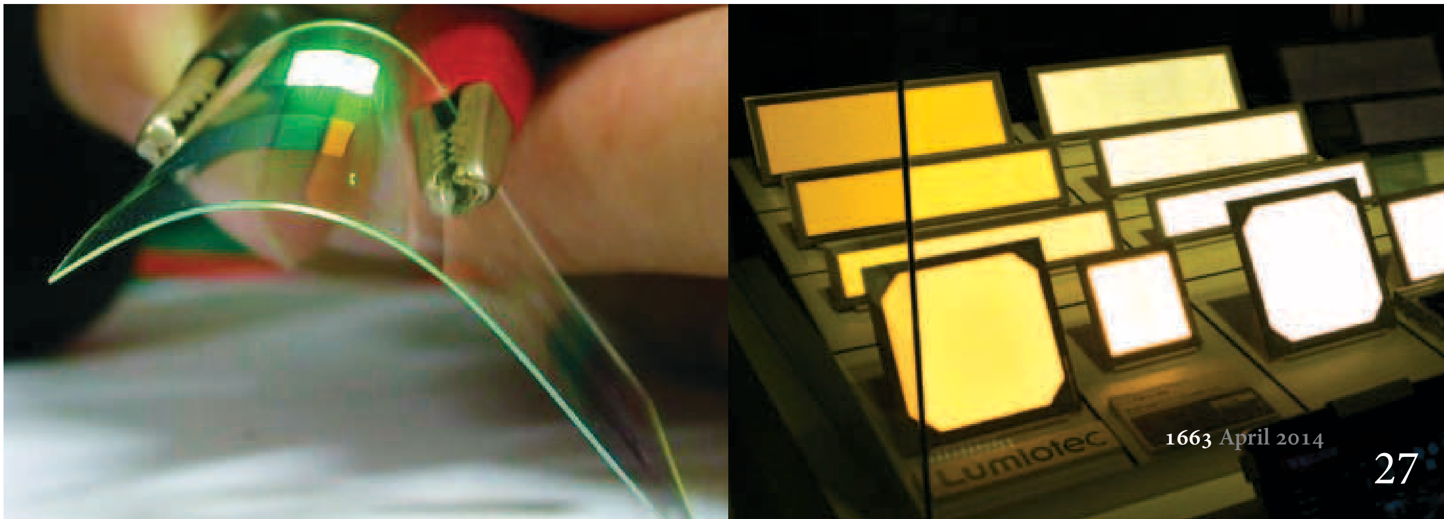
—*Craig Tyler*

Brighter Future for Cancer Detection

What do high-speed communication, advanced microscopy, high-tech security systems, and noninvasive cancer detection have in common? They are all made possible by fiber optics. Los Alamos researcher Judith Mourant is a light scattering expert using fiber optics to pioneer a new method to detect cervical cancer. Cervical cancer is still a common cancer for American women, despite an enormous decrease in incidence since the implementation of regular screening in the 1950s. After initial screening via the Papanicolaou test (a.k.a. Pap smear), abnormal or suspect findings are subjected to more sensitive diagnostic procedures, primarily colposcopy (illuminated magnification) and biopsy (tissue sampling). Biopsies are small portions of tissue and their removal (typically by scalpel or laser) can cause pain, infection, or other complications. Combine this with the stress of waiting for results, and some patients wind up avoiding the procedure until it may be too late. Furthermore, biopsies can only sample a small portion of the tissue. To improve this, Mourant and her team developed a noninvasive fiber-optic method that can improve the process of choosing when and where to biopsy that could eventually decrease both the cost of detection and stress to patients.

Mourant, along with former Los Alamos cell biologist James Freyer, previously showed that cancerous cells scatter light differently than noncancerous cells. When you hold a flashlight against your palm in a dark room, your hand will glow red. The red color is because your tissue absorbs the other colors of light, especially blue and green, while the red light, reflected off your blood cells, passes through. But it doesn't go straight through the tissue of your hand—it is scattered, or bounced around, by microscopic structures it encounters along the way. When light bounces off of structures in tissue, the change in intensity of the scattered light can be quantified and used to infer information about the physical properties and structure of the tissue.

After proving her method in laboratory-cultured cells, Mourant and her colleagues



A flexible OLED device (left) and prototype OLED lighting panels

CREDIT: meharris (left) and STRONGlk7/Wikimedia Commons packaged it into a safe and compact fiber-optic probe-based system that can be used during routine patient examination. Clinical trials performed in collaboration with researchers at the University of New Mexico Health Science Center and the Albert Einstein College of Medicine in New York compared the fiber-optic system against traditional colposcopy. Initial tests showed that the optical system has similar accuracy for the detection of precancerous lesions to that of well-trained and experienced colposcopists.

Presently, Mourant and Los Alamos technologists Oana Marina and Claire Sanders are trying to determine what specific molecular changes within the cell are responsible for the differences in light scattering, and they are looking at the potentially helpful effect of acetic acid. Topical application of acetic acid (the main component of vinegar) often causes cancerous and precancerous cells to visibly whiten and is regularly used during colposcopy. The problem with the acetowhitening-colposcopy system is that it relies on the human eye (the eye of whichever clinician is performing the exam), which permits neither quantification nor standardization. The whitened appearance is actually an increase in the amount of light reflecting from the tissue's surface, prompting Mourant to speculate that the molecular mechanism responsible for acetowhitening may also be involved in the light scattering differences exploited by her optical diagnostic system. If they can determine which cellular elements are scattering the most light, and whether these are the elements that are altered during cancer, they may be able to apply their analysis to other types of tissue and their corresponding cancers.

Determining properties of tissue by measuring the intensity of light that has passed through it is difficult, because it is hard to know where the light went without already knowing the detailed structure of the tissue. One approach to this problem is to simulate light transport through tissues with slightly different, predefined properties. To do this, Mourant has teamed up with Jerome Spanier and his team of mathematical modelers at the University of California at Irvine to develop computational methods to simulate light passing through different types of tissues. By bringing together cellular systems, optical systems, mathematical modeling, and high-performance computing, this technology will improve both the clinical experience and the accuracy of diagnosis.

Moving forward, Mourant sees this work being relevant to many other questions in cancer biology. "Using fiber optics to look at the insides of people is not new to medicine. But we are not just looking, we are diagnosing. And that is new and very exciting," she says. In fact, the diagnostic power of fiber optics is also being investigated by other research groups studying colon and esophogeal cancers, which frequently reach late-stage disease before diagnosis, have high mortality rates, and cost billions annually to treat. Indeed, just as high-speed communication and other modern conveniences have benefitted from fiber optics, so too may certain essentials of health and longevity.

—*Eleanor Hutterer*

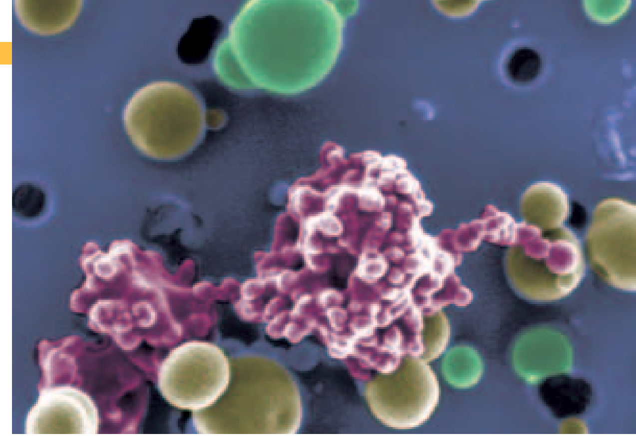
The probe used during a clinical exam for fiber-optic detection of cervical cancer is about 3 millimeters in diameter.

Warming by Wildfire?

Here's the thing about predicting the climate: it's all based on models. Models are built with the pieces you have, and you need the right pieces to get the right prediction. According to Los Alamos climate scientist and emissions expert Manvendra Dubey, the models currently being used to simulate and predict climate change may not have all the right pieces when it comes to wildfires.

When the record-breaking Las Conchas megafire came to Los Alamos's doorstep in June of 2011, Dubey saw an opportunity for discovery. The town had been evacuated at the peak of the threat, but once the fire was reduced to a smolder and the evacuation order was lifted, Dubey and his team hurried to deploy aerosol emissions sensors. They wanted to know what kind of carbon particles were in the air after such a large, hot fire. The size and shape of the collected particles were examined by electron microscopy, and the results were startling.

The majority of collected particles were amorphous, spherical carbon particles called



False-color scanning electron micrograph showing aerosol particulates collected from Los Alamos after the Las Conchas megafire in 2011. Three types of carbon particles are shown: climate-cooling dark tarballs (green), climate-warming bright tarballs (soft yellow), and an aggregated clump of organic-coated soot particles (pink).

tarballs. These can have either a warming or cooling effect on climate, depending on whether they absorb or scatter sunlight, but are not normally taken into account in climate models because they aren't considered significant. The team expected to see some tarballs in their analysis, but they saw a lot— in fact, the tarballs were the dominant type of particle. Another surprise was that there were two kinds of tarballs—dark and bright—visible in the electron microscopy images. The team, which included Claudio Mazzoleni of Michigan Technological University (formerly a Los Alamos Director's postdoctoral fellow mentored by Dubey), found that dark tarballs, which comprise about a third of the tarballs examined, are more highly oxidized than bright tarballs. Highly oxidized organics like these are more efficient than less-oxidized organics in taking up water to become cloud drops—the tiny droplets of water that largely make up a cloud. By increasing the number, size and concentration of these drops within a cloud, the presence of dark tarballs, counterintuitively, makes the cloud reflect more sunlight, resulting in a cooling effect.

Dubey also found another surprise in the Las Conchas fire emissions analysis, this one involving soot particles—small spherical particles of black carbon that aggregate together in chain-like clumps. Most of the soot particles examined were coated with other organic compounds from the fire—compounds that focus sunlight, resulting in a warming effect. This means that soot particles, which are treated as bare in most climate models, are being modeled incorrectly because the organic coating alters their optical (light absorbing or reflecting) and physical-chemical (aerosol-cloud interaction) properties. At the time, the Las Conchas fire was the largest in New Mexico history (156,000 acres); however, the following year the Whitewater-Baldy Complex fire became the new record holder (289,000 acres), and Dubey's team confirmed their dark tarball and coated-soot findings from that fire as well.

Emissions from burning biomass include both light-absorbing particles (soot and black carbon) as climate warmers and light-scattering particles (organic carbon and smoke) as climate coolers. Current climate models typically indicate small wildfire contributions to climate because they assume that the warming particles and cooling particles offset each other's effect. Dubey's work has shown that not only is the composition of carbon-based aerosols more complex than previously realized, but the relative warming and cooling contributions of each of these types of particles do not necessarily cancel: warming can win.

Dubey concludes that global climate models, which only include organic aerosols (cooling) and bare soot (warming), ought to include both kinds of tarballs (warming and cooling) as well as soot coated with organics (more warming than bare soot). Punctuating this recommendation is the rising incidence of record-breaking wildfires in New Mexico, the American Southwest, and the rest of the world. It is a ferocious feedback loop: as the climate warms from greenhouse gas emissions, fires will be larger, hotter, and more frequent and will emit an abundance of tarballs and soot. The next challenge is to determine just how much warming is actually canceled by cooling. According to Dubey, it may be less than we thought. LDRD

—*Eleanor Hutterer*

Supernova for National Security

What Los Alamos astrophysicist Chris Fryer realized as he looked at the latest NuSTAR images of Cassiopeia A (Cas A) was that, in a curious way, the country had just been handed a windfall. Cas A is a supernova remnant—the stellar debris that remains after the core of a supermassive star implodes and gives birth to a neutron star, but then explodes and blows the rest of the star apart. NuSTAR is NASA's high-energy x-ray telescope that had been mapping the location of titanium nuclei in the still-expanding debris field, now some 10 light-years across. The windfall, however, begins with NuStar's older brother spacecraft, the Chandra X-ray Observatory.

"The Cas A debris field is turbulent," says Fryer, "and over the course of several years, Chandra captured beautiful images of turbulent mixing. We hoped we could use the images to test our computer codes, but that wasn't possible at the time."

Every computer simulation of a supernova includes code that accounts for turbulence in the core and body of the star. But is that code correct, and are the physics models that describe the turbulence correct or even adequate? The only way to be sure is to simulate the system and compare its output turbulence with the signature swirls, whorls, and plumes displayed by the real system. However, the swirls and whorls seen in Cas A today are in part due the shape of the star's core when it blew up. That shape was unknown, and thus there was too much uncertainty in the simulation to deduce if it reflected reality or not.

Interestingly, turbulence also shows up in another system that first implodes then explodes—the plutonium core of a nuclear weapon. Like the astrophysicists, weapons scientists need to validate and verify their computer codes that model weapons performance. Unfortunately, it is extraordinarily difficult to obtain data that could be used to test the weapons code. Fryer had proposed using the Cas A data.

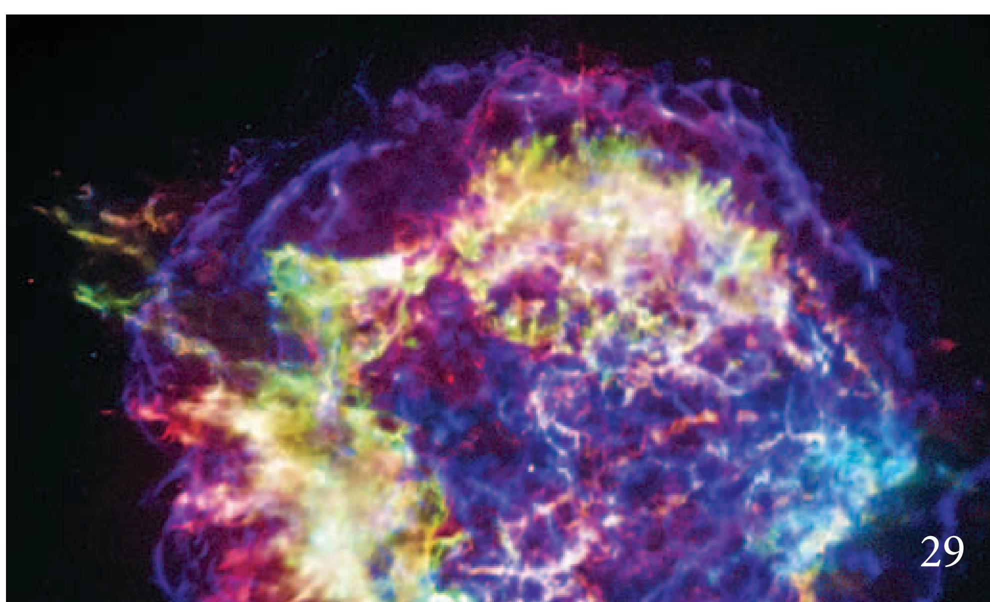
Wait a minute. Why should the turbulence within a supernova remnant 10 light-years across have anything to do with the turbulence of a detonated nuclear device? The answer is that the underlying physics is the same—and the physics governs the type of turbulence that emerges within each system.

"We've been able to learn more about how to model a nuclear weapon by modeling supernovae," says Fryer.

Supernovae are perhaps the best examples of how basic science, the cornerstone of the U.S. and the world's technological powerhouses, can support the weapons program. But it's not the only example. In many specialized areas of science, where the expertise has traditionally resided behind the security fence, the much larger peloton of academic and private-sector scientists has closed the gap in basic knowledge, and as Fryer sees it, has a lot to offer the secretive and traditionally self-contained world of nuclear weapons.

Fryer has ties to both the academic and weapons communities. As a member of NuSTAR's science team, he's privy to the telescope's data. The titanium nuclei that were being mapped are only created in the core of a massive star and thus serve as markers for core material. What caught his eye was that the nuclei were distributed in a way that was entirely consistent with the latest models of core collapse and explosion. That meant that astrophysicists had a handle on the shape of the core that created Cas A and could estimate the uncertainties in reproducing the turbulence observed by Chandra. And that weapons scientists could to do similar tests with their codes using the Chandra data—for free. LDRD

—*Jay Schecker*



A composite image of the supernova remnant Cassiopeia A, combining low-energy (red), medium-energy (green), and high-energy (blue) x-ray images taken by the Chandra X-ray Observatory. The tiny bright dot in the center is believed to harbor a neutron star.

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